

Genetic and Proteomic Analyses of Pupylation in *Streptomyces coelicolor*

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Strains, Media and Culture Conditions. *Streptomyces coelicolor* strains were grown at 30°C on mannitol soy flour medium (SFM), Difco nutrient agar medium (DNA), yeast extract-malt extract medium (YEME), or Tryptone Soya Broth (TSB). SFM was used for conjugations between *S. coelicolor* and *Escherichia coli* and for generating spore stocks. *Escherichia coli* strains DH5 α and ET12567/pUZ8002 were grown on Luria-Bertani medium at 37°C for routine subcloning. For the selection of *E. coli*, ampicillin, apramycin, chloramphenicol, hygromycin, and kanamycin were employed at 100, 50, 25, 80, and 50 μ g/ml, respectively. Nalidixic acid was used at 20 μ g/ml to counterselect *E. coli* in conjugations with *S. coelicolor*. Apramycin and hygromycin were used at 50 μ g/ml for the selection of *S. coelicolor* exconjugants.

Table S1: Strains used in this study

Strain	Description	Source/Reference
<i>Streptomyces coelicolor</i>		
M145	Prototroph SCP1-, SCP2-	--
B1643	M145 Δ 1643-1644::apr	This Study
B1646	M145 Δ 1643-1646::apr	This Study
B1640	M145 Δ 1640::apr	This Study
B1647	B1646 - pJS873	This Study
B1648	B1640 - pJS873	This Study
B1649	M145 WT - pMS81	This Study
B1650	B1646 - pMS81	This Study
B1651	B1640 - pMS81	This Study
B1640c	B1640 - pJS877	This Study
B1652	B1646 - pJS875	This Study
<i>Escherichia coli</i>		
DH5 α	F- φ 80lacZ Δ M15 Δ (lacZYA-argF) U169 recA1 endA1 hsdR17 (rK- mK-) phoA supE44 thi-1 gyrA96 relA1 λ dam, dcm, hsdS, cat, tet	Invitrogen
ET12567	Δ (araD-araB)567	1
BW25113	Δ lacZ4787(:rrnB-4) lacIp-4000(lacIQ), λ , rpoS369(Am), rph-1, Δ (rhaD-rhaB)568, hsdR514	1

Standard cloning procedures were employed in generating the plasmids listed in Table S2. The site-specific integrating vector pMS81 was used for genetic complementation as previously described (1). DNA sequencing was performed by Davis Sequencing (Davis, California). Table S3 shows the primers used in this work, all of which were synthesized by Invitrogen. PCR was performed with *Taq* (Invitrogen) and *Pfu* (Stratagene, Agilent Technologies). All PCRs were performed with 5% (vol/vol) dimethylsulfoxide (DMSO).

Table S2: Plasmids used in this study

Plasmid	Description	Source/Reference
pIJ790	[oriR101], [repA101(ts)], araBp-gam- bet-exo, Chl ^R	1
pUZ8002	RP4 Derivative, OriT-, Kan ^R	1
pMS81	OriT, ϕ BT1 attB-int, Hyg ^R	1
pBlueScript KS+	pUC ori, MCS, AmpR	Agilent Technologies (Stratagene)
pIJ10257	oriT, ϕ BT1 int-attB, hyg, ermEp*	2
His tagged Pup fragment (258bp) in pBS pMA-RQ	oriCol E1, synthetic <i>Sco</i> Proteasome, AmpR	Genewiz
pJS868	Sti41 Δ 1647::apr	This Study
pJS869	Sti41 Δ 1643-1644::apr	This Study
pJS870	Sti41 Δ 1640::apr	This Study
pJS871	Sti41 Δ 1643-1646::apr	This Study
pBlueScript -EarI	pUC ori, MCS AmpR, -EarI sites	This Study
pJS872	258 bp synthetic fragment from pMA-RQ + 2671 bp SexAI and SphI fragment containing <i>sco1643-1646</i> in pBlueScript - EarI	This Study
pJS873	<i>Sco 1643-46</i> subcloned from pJS872 into pMS81 using EcoRV and SpeI	This Study
pJS874	1232 bp <i>Sco 1645-46</i> pcr amplified from pJS872 and subcloned into pBS	This Study
pJS875	<i>Sco 1645-46</i> subcloned from pJS874 into pMS81 using EcoRV and SpeI	This Study
pJS876	3141 bp NotI and AluI fragment containing <i>sco1640</i> in pBlueScript KS+	This Study
pJS877	<i>Sco1640</i> subcloned into pMS81 from pCC1640b using EcoRV and SpeI	This Study

Table S3: Primers used in this study

Primer Name	Application/Function	Sequence
Sco 1643-46 KO F (+SpeI)	PCR targeting/disruption of <i>sco1643-46</i>	CCCGGCTGCACCTCGTCGACCTTCAGTACGC CGACGTAC actagt ATTCCGGGGATCCGTGACC
Sco 1643-46 KO R (+SpeI)	PCR targeting/disruption of <i>sco1643-46</i>	CACGATGCGCTTGAACTTGCCTGCTGCCG ACGCGTCCG actagt TGTAGGCTGGAGCTGCTTC
Syn. Pup His seq. 1	Sequencing primer for His-tagged <i>sco1646</i>	GTGAGGGTTATGCACCAACCACCAACCAC

Syn. Pup His seq. 2	Sequencing primer for His-tagged <i>sco1646</i>	CTTCAAACAAATCACCGAGAG
SCO 1640 KO F (+Spel)	PCR targeting/disruption of <i>sco1640</i>	GTCATGGACCGCCGCATTTGGGCTGGAG AACGAGTAC actagt ATTCCGGGGATCCGTGACC
SCO 1640 KO R (+Spel)	PCR targeting/disruption of <i>sco1640</i>	GTCGTCCACCGAACCGAACGGTCTTGCA CAACACGG Tactagt TGTAGGCTGGAGCTGCT TC
SCO 1643 KO F (+Spel)	PCR targeting/disruption of <i>sco1643-1644</i>	GTCAACGGCCCCGCCGATGAGGTGAGGT GAGCGCCTA actagt TGTAGGCTGGAGCTGCT TC
SCO 1643 KO R (+Spel)	PCR targeting/disruption of <i>sco1643-1644</i>	GGGCGTCTACCAGCTGCCTTCCTGACGCCG GGTCCTCA actagt ATTCCGGGGATCCGTGCA CC
SCO 1647 KO F (+Spel)	PCR targeting/disruption of <i>sco1647</i>	AGCGCAAAGGCGTTCTAGGCTCTTCATAC CGCCGAGTC actagt ATTCCGGGGATCCGTGCG ACC
SCO 1647 KO R (+Spel)	PCR targeting/disruption of <i>sco1647</i>	GCAGCGGTCCAGGAGCTCCTTGACGTGATT ACGCGTTCC actagt TGTAGGCTGGAGCTGCT TC
SCO 1643- 1644 KO Detect F	Verification of <i>sco1643-1644</i> replacement with <i>apr</i>	GCACTTGAAGCGTCACTACG
SCO 1643- 1644 KO Detect R	Verification of <i>sco1643-1644</i> replacement with <i>apr</i>	CGACGACGACAAACTGGCG
SCO 1647 KO Detect F	Verification of <i>sco1647</i> replacement with <i>apr</i>	TGTACATCCGTACGCTCGTC
SCO 1647 KO Detect R	Verification of <i>sco1647</i> replacement with <i>apr</i>	GACACAGTTGCTCGGTCAAG
SCO 1643- 1646 KO Detect F	Verification of <i>sco1643-1646</i> replacement with <i>apr</i>	CGACGACCAAGGAC
SCO 1643- 1646 KO Detect R	Verification of <i>sco1643-1646</i> replacement with <i>apr</i>	CATCGACCCCGAACTCAC
SCO 1640 KO Detect F	Verification of <i>sco1640</i> replacement with <i>apr</i>	GTCTCGCTGCTCGTACTG
SCO 1640 KO Detect R	Verification of <i>sco1640</i> replacement with <i>apr</i>	ACGGCGA TGAGGAGTGAG
Sco 1645-46 Clone F	Amplification of <i>sco1645-46</i> with His ₆	CTCCTGGACTCGGTGATC
Sco 1645-46 Clone R	Amplification of <i>sco1645-46</i> with His ₆	CTCCGGCTGGTGTAC
C519G (F)	Site-directed mutagenesis primer for pBlueScript KS+ to generate pBlueScript -Earl	TCGGTGCGGGCTCTGGCTATTACGC
C519G (R)	Site-directed mutagenesis primer for pBlueScript KS+ to generate pBlueScript -Earl	GCGTAATAGCCAAGAGGCCGCACCGA
C1036G (F)	Site-directed mutagenesis primer for pBlueScript KS+ to generate pBlueScript -Earl	GTATTGGCGCTTGCCTTCCCGC
C1036G (R)	Site-directed mutagenesis primer for pBlueScript KS+ to generate pBlueScript -Earl	GCGAGGAAGCCAAAGAGC GCCCAATAC
T2836A (F)	Site-directed mutagenesis primer for pBlueScript KS+ to generate	CACGGAAATGTTGAATACTCATACACTTC

T2836A (R)	pBlueScript -Earl Site-directed mutagenesis primer for pBlueScript KS+ to generate pBlueScript -Earl	CTTCAATAATATTGAAAAAGGAAGTGTAT
SCO 1640+NdeI F	Overexpression of <i>sco1640</i>	CATATGGACCGCCGCATTTTC
SCO 1640+HindIII R	Overexpression of <i>sco1640</i>	AAGCTTCACATCCGGCC AT

Construction of *PPS* (*SCO1643-46*), *prc* (*SCO1643-44*) and *pafA* (*SCO1640*) null mutants. Strains of *S. coelicolor* in which either the *pps* locus (*SCO1643-46*), the *prc* (*SCO1643-44*) or the *pafA* locus (*SCO1640*) were replaced with an apramycin (*apr*) resistance cassette were constructed via polymerase chain reaction (PCR)-targeted mutagenesis (3). The *apr* resistance cassette for replacement of the *PPC* was prepared using PCR primers SCO1643-46 KO FOR and SCO1643-46 KO REV and the Expand High Fidelity DNA polymerase (Roche). The *apr* resistance cassette for replacement of *pafA* was prepared using the Expand High Fidelity polymerase (Roche) and PCR primers SCO1640 KO FOR and SCO1640 KO REV. The *apr* resistance cassette for replacement of *prc* was prepared using the Expand High Fidelity polymerase (Roche) and PCR primers SCO1643 KO FOR and SCO1644 KO REV. (Table S3). The resistance cassettes were introduced individually into *E. coli* BW25113/pIJ790 containing the appropriate WT (StI41) cosmid. Arabinose was added to induce expression of the λ RED recombinase. The resulting recombinant cosmids, StI41 ΔSCO1643-46::*apr* (pJS871), StI41 ΔSCO1643-44::*apr* (pJS869), and StI41 ΔSCO1640::*apr* (pJS870), were transformed into ET12576/pUZ8002, a non-methylating strain of *E. coli*, and introduced into wild-type *S. coelicolor* A3(2) M145 through conjugation as previously described (3), yielding *S. coelicolor* B1646, B1643, and B1640, respectively. Double cross-over exconjugants were selected by apramycin resistance and kanamycin sensitivity. The disruption of *SCO1643-46*, *SCO1643-44* and *SCO1640* were confirmed via PCR on isolated genomic DNA from *S. coelicolor* using the appropriate KO Det primers (Table S3).

Complementation of *ΔpafA*. A 3141-bp fragment was excised from cosmid StI41 containing the *sco1640-1* ORFs, 250 bp upstream of the *sco1641* translational start site, and 302 bp downstream of the *sco1640* translational stop by restriction digestion with NotI and MluI. The fragment was treated with DNA polymerase I Large (Klenow) Fragment (New England Biolabs). The blunt-ended fragment was then ligated into the SmaI site of pBlueScript KS+ to yield pJS876. The fragment containing the *sco1640-1641* locus was excised and ligated into pMS81 using EcoRV and SpeI restriction digestion to yield pJS877. pMS81 is a site-specific integrating vector that inserts into the ΦBT1 attB site of *S. coelicolor*. (1) pJS877 was transformed into ET12576/pUZ8002 and introduced into *S. coelicolor* via conjugation, yielding strain *B1640c*. Ex-conjugants were selected based on hygromycin resistance.

Construction of Affinity-tagged Pup. For identification of pupylated targets in *S. coelicolor*, an His-tagged version of Pup was constructed. To maintain the

endogenous regulation mechanisms, instead of using a His₆-tagging expression vector, we utilized a synthetic fragment of the N-terminus of the *pup* gene to which a hexahistidine sequence had been added after the initiator ATG (synthesized by Genewiz). Using unique restriction sites SexAI and EarI, the 258 bp synthetic fragment was transferred to the corresponding location on a pBlueScript KS+ clone carrying a 2933 bp Stl41-derived fragment containing the *SCO1643-1646* locus. Prior to fragment transfer, three rounds of site-directed mutagenesis (QuickChange protocol) were carried out on pBlueScript to ablate its three EarI sites. Additionally, digestions using SexAI were carried out in *E. coli* ET12567/pUZ8002 (dam⁻), since the SexAI site is blocked by methylation in dam⁺ hosts. After successful ligation into the pBlueScript backbone and confirmation of the construct by sequencing (Davis Sequencing), the synthetically modified *sco1643-1646* locus was transferred to pMS81 (pJS873) and conjugated with *S. coelicolor* strain B1646 *S. coelicolor*. This construct has a fully functional *prc* locus.

To analyze pupylated targets in an *S. coelicolor* strain lacking the *prc* locus, we used primers *SCO1645-46* clone F and *SCO1645-46* clone R to amplify the His-tagged *pup* from pJS872. The PCR-amplified locus was cloned into the SmaI site of pBS-KS+, transferred to PMS81, and conjugated into *S. coelicolor* strain B1646. This construct has a His-tagged *pup* but lacks a functional *prc* locus.

Antibiotic Production and Sporulation Analysis. To assess phenotypic differences of *S. coelicolor* strains, 10⁶ spores were grown as a lawn on divided SFM plates at 30°C and monitored over 90 hrs for visible differences in spore formation and antibiotic production (color change to blue or red pigment indicating actinorhodin or undecylprodigiosin production).

Figure S1. Phenotype of *S. coelicolor* null mutants.

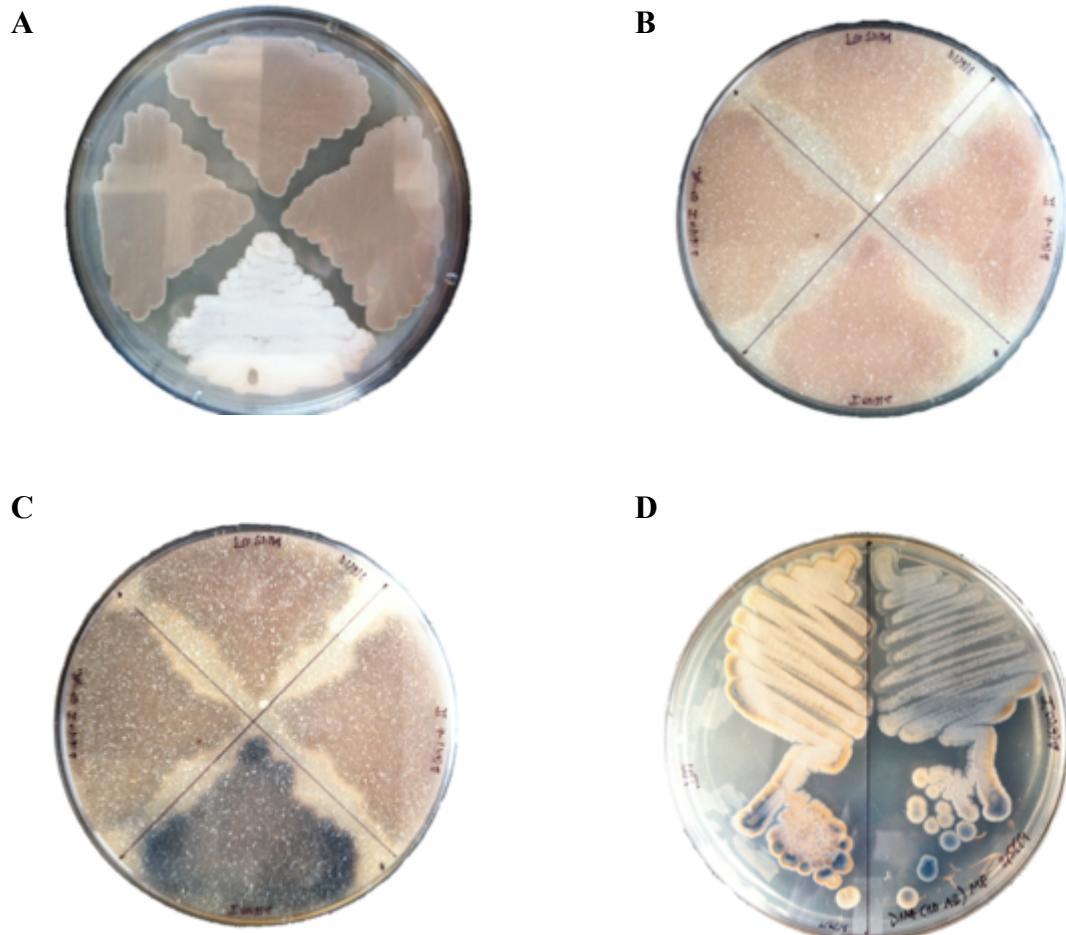


Figure S1. (A) $\Delta pafA$ exhibits sporulation defects. Clockwise from bottom: $\Delta pafA$, $\Delta 1643-1646::apr$, WT M145, $\Delta pafA$ complemented. Growth on SFM after 30 hours. **(B) $\Delta pafA$ and $\Delta 1643-1646::apr$ exhibit overproduction of undecylprodigiosin.** Clockwise from bottom: $\Delta pafA$, $\Delta pafA$ complemented, WT M145, $\Delta 1643-1646::apr$. Growth on SFM for 70 hours. **(C) $\Delta pafA$ exhibits overproduction of actinorhodin.** Clockwise from bottom: $\Delta pafA$, $\Delta pafA$ complemented, WT M145, $\Delta 1643-1646::apr$. Growth on SFM for 90 hours. **(D) $\Delta pafA$ actinorhodin phenotype is replicated on nutrient-rich media.** Left: WT M145, right: $\Delta pafA::apr$. Growth on DNA for 90 hours.

Heat Inactivation of Spores. To determine if spores were susceptible to heat, an equal amount of spores of WT and *pafA* null strains of *S. coelicolor* (1×10^8) were incubated for either 0, 10, 20, 30, 40, 50, or 60 minutes at 55°C in 20 % glycerol. After incubation, the spore stocks were diluted, plated on Difco Nutrient Agar and the colonies were tallied. The values depicted are the average of three replicates.

Figure S2. Heat Inactivation of *S. coelicolor* Spores

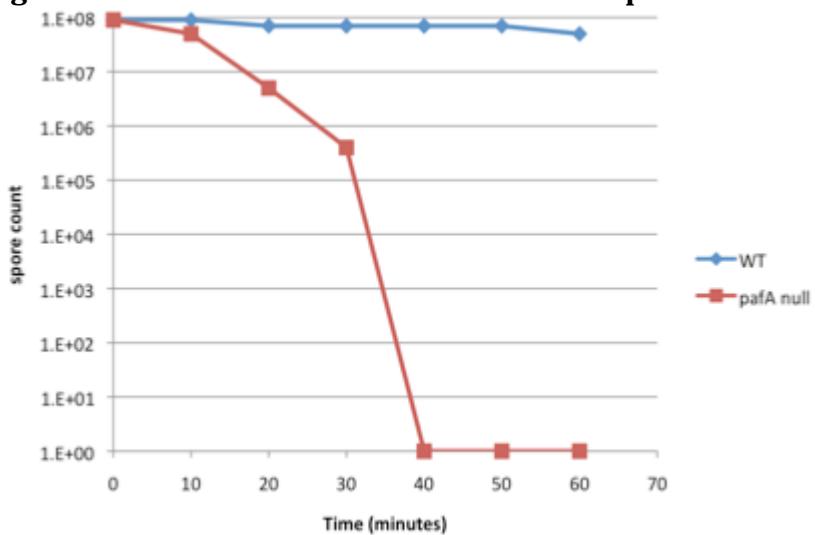


Figure S2. Heat Inactivation of *S. coelicolor* WT and *pafA* null strain spores.
Spores were incubated at 55°C for varying amounts of time and spore titres
were determined.

Oxidative Stress Assay. In assessments of the strains' sensitivities to oxidative stress, equal numbers of spores of the wild-type, $\Delta prc::apr$, $\Delta pps::apr$, $\Delta pafA::apr$, $\Delta pafA::apr$ complemented, $\Delta pps::apr$ with pJS872 (HisPup) (1×10^8) were plated on either SFM or DNA. To the center of each freshly inoculated plate was added a sterilized and dry paper disc (6mm diameter) that had been submerged in a 40% solution of cumene hydroperoxide in dH₂O. After growth at 30°C for 48 hrs on DNA or 72 hrs SFM, the size of the cleared zone was measured. These experiments were replicated 4 times and the average sizes of the zones of inhibition are reported.

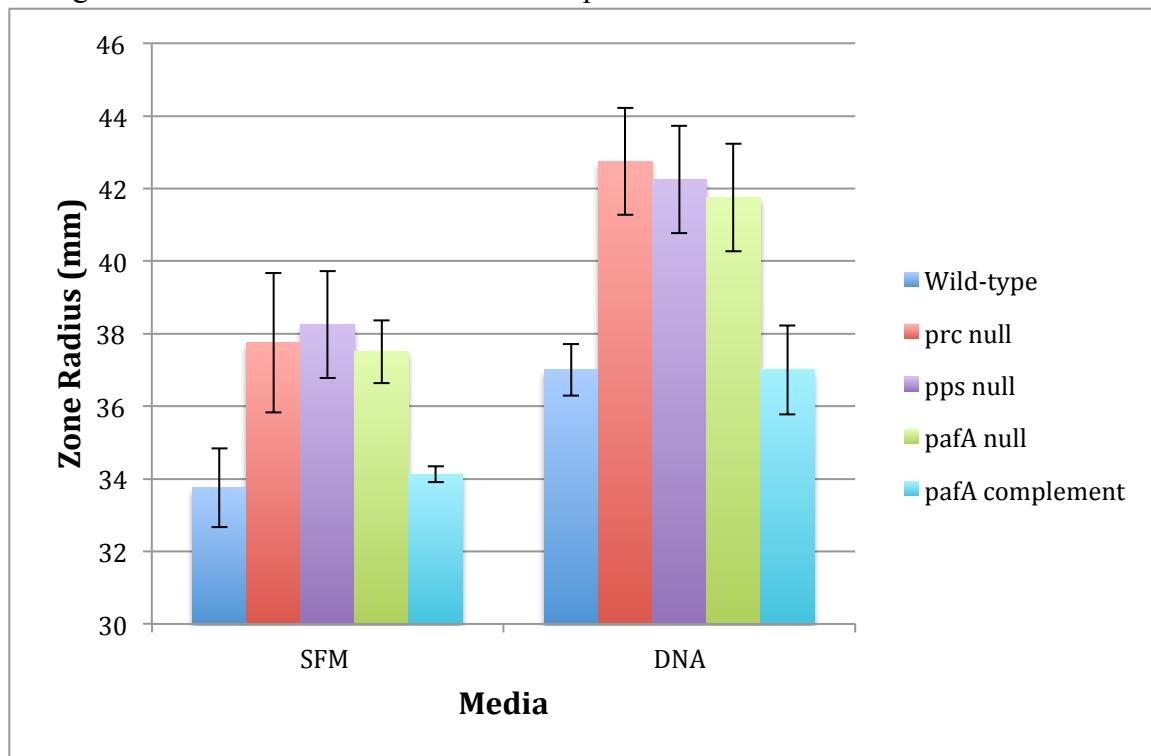


Figure S3. Cumene hydroperoxide sensitivity of *S. coelicolor* strains as measured on SFM or DNA. Errors bars represent standard deviation.

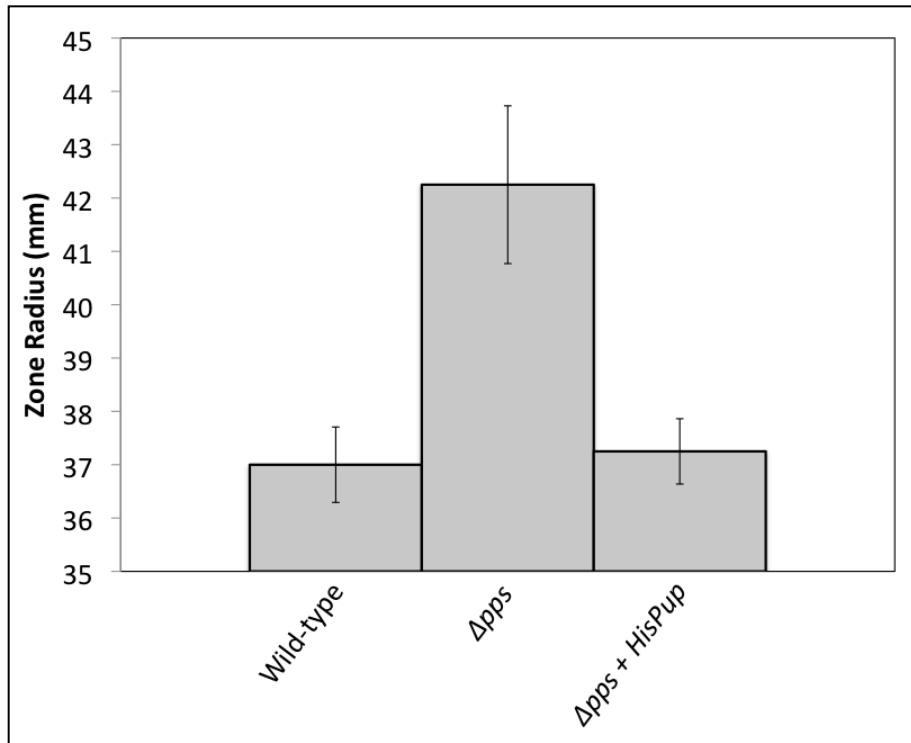


Figure S4. The His-tagged Pup is fully functional. Cumene hydroperoxide sensitivity of *S. coelicolor* wild-type, Δpps , and $\Delta pps + \text{pJS873}$. pJS873 contains the full *pps* with a N-terminally hexa-histidine tagged *pup*. These experiments were performed on DNA and the error bars represent the standard deviation.

Purification of Pupylated Substrates. Shaken, liquid cultures (50mL) of *Streptomyces coelicolor* were grown until either early exponential, late exponential, or stationary growth phase and harvested by centrifuge at 4000rpm for 10 minutes. The cell pellets were resuspended in 1.4mL lysis buffer (50mM NaH₂PO₄, 300mM NaCl, 10mm Imidazole, pH 8.0). and 4.5µL 1:9 benzonase buffer (50mM Tris-HCl, 20mM NaCl, 20mm MgCl₂, pH 8.0). For lysis, lysozyme was added to a final concentration of 1 mg/mL. After incubation on ice for 1 hour, cells were lysed by sonication at 60% power three times at 30-second intervals with 2 minutes of rest between each sonication. Lysates was clarified at 4°C by centrifugation at 13,000 rcf, after which affinity-tagged proteins were isolated using the Qiagen Ni-NTA column purification kit following manufacturer's protocol. Two protein samples from each strain were isolated in this fashion and subjected to peptide mass fingerprinting.

Protein Identification via Mass Spectrometry and Bioinformatics. For the identification of proteins captured by the Ni-NTA columns, the eluates were tryptically digested. The resulting peptides were loaded onto a reverse phase column and separated by an Agilent 1200 HPLC. The peptides were identified by tandem, high-resolution MS/MS analyses using a coupled LTQ Orbitrap Velos mass spectrometer at the Brown University Center for Genomics and Proteomics. The mass spectral data were searched using the MASCOT software algorithm against the corresponding bacterial protein database. Modification of lysine residues to incorporate 243 Daltons from Pup was required as a search criterion. In the bioinformatic identifications of the peptide fragments, trypsin specificity with two missed cleavage sites was allowed and the MS mass tolerance was 7 ppm while the MS/MS tolerance was 0.5 Da. Identifications were contingent on at least one unique peptide spectrum match (PSM) in the molecular weight search (MOWSE) with a protein score cutoff of 1. All proteins identified are listed in Tables S4-S6.

Table S4 – Proteins identified to be pupylated in an early exponential stage growing culture.

Pupylated Proteins Identified in Early Exponential Growth					
Wild-Type			<i>Aprc::apr</i>		
2-amino-3-ketobutyrate coenzyme A ligase (SCO 6800)	Clp A (SCO 6408)	PhoH-like protein (SCO 2532)	30S Ribosomal protein S7 (SCO 4660)	Methyltransferase (SCO 2317)	
30S Ribosomal protein S12 (SCO 4659)	Cob(I)alamine adenosyltransferase (SCO 1851)	Polyphosphate kinase (SCO 4145)	5'-Nucleotidase (SCO 4152)	Heat Shock Protein, DnaK (SCO 3671)	
30S Ribosomal protein S13 (SCO 4727)	DNA gyrase subunit B (SCO3874)	Protease (SCO 5838)	Aconitate hydratase (SCO 5999)	Oligopeptide-binding lipoprotein (SCO 5477)	
30S Ribosomal protein S7 (SCO 4660)	Elongation factor P (SCO 1491)	Protein kinase, pglW (SCO 6626)	Allantoate amidohydrolase (SCO 3072)	Oxidoreductase (SCO 7572)	
5'-Nucleotidase (SCO 4152)	Elongation factor Ts (SCO 5625)	Reductase (SCO 1229)	DNA ligase (SCO 6707)	Protein kinase, pglW (SCO 6626)	
50S Ribosomal protein L15 (SCO	Gamma-glutamyl kinase (SCO 2587)	Serine protease (SCO 2637)	RNA helicase (SCO 4096)	pseudouridine synthase (SCO	

4721)				1768)
50S Ribosomal protein L4 (SCO 4703)	Glucarate dehydratase (SCO 2542)	Succinate dehydrogenase iron-sulfur subunit (SCO 4855)	Bifunctional alpha-amylase/dextrinase (SCO 2226)	Regulatory protein (SCO 3664)
50S Ribosomal protein L6 (SCO 4717)	Glycerol-3-phosphate dehydrogenase (SCO 5559)	Transcriptional regulator (SCO 1463)	GroEL (SCO 4296)	Succinyl-CoA synthetase subunit beta (SCO 4808)
6-Phosphofructokinase (SCO 1214)	GTP-binding protein (SCO 5111)	Transcriptional regulator (SCO 3571)	Clp A (SCO 6408)	Tellurium resistance protein (SCO 4277)
Acetyltransferase (SCO 1563)	Histidyl-tRNA synthetase (SCO 1508)	Translation initiation factor (SCO 3014)	DNA gyrase subunit B (SCO 3874)	Transcriptional regulator (SCO 3571)
Aconitate hydratase (SCO 5999)	Hydrolase (SCO 4323)	Urease alpha subunit (SCO 1234)	DNA integrity scanning protein DisA (SCO 3352)	Translation initiation factor (SCO 3014)
Acyl-CoA dehydrogenase (SCO 6469)	Nucleotidyltransferase (SCO 3122)		DNA topoisomerase (SCO 6517)	Valine dehydrogenase (SCO 4089)
Adenylosuccinate synthetase (SCO 3629)	Oligopeptide-binding lipoprotein (SCO 5477)		Enoyl-ACP reductase, inhA (SCO 1814)	
Aminopeptidase (SCO 2635)	Oxidoreductase (SCO 7572)		Glucarate dehydratase (SCO 2542)	
Cellulose-binding protein (SCO 5396)	Peptidase (SCO 0432)		Indole-3-glycerol-phosphate synthase (SCO 2039)	

Table S5 – Proteins identified to be pupylated in a late exponential stage growing culture.

Pupylated Proteins Identified in Late Exponential Growth				
Wild-Type		<i>Aprc::apr</i>		
ABC transporter ATP-binding protein (SCO 6454)	Oxidoreductase (SCO 7572)	30S Ribosomal protein S3 (SCO 4708)	Nitrite/sulfite reductase (SCO 6102)	
Acetyl/propionyl CoA carboxylase beta subunit (SCO 2776)	PhoH-like protein (SCO 2532)	50S Ribosomal protein L2 (SCO 4705)	Oxidoreductase (SCO 7572)	
Aldoketoreductase (SCO 4951)	Preprotein translocase (SCO 3005)	Aconitate hydratase (SCO 5999)	PhoH-like protein (SCO 2532)	
Aldolase (SCO 1087)	Prolyl-tRNA synthetase (SCO 5699)	Aspartate aminotransferase (SCO 4645)	Protease (SCO 5838)	
D-3-phosphoglycerate dehydrogenase (SCO 5515)	Protein kinase, pgIW (SCO 6626)	Cell division protein FtsH homolog (SCO 3404)	Pseudouridine synthase (SCO 1768)	
Deoxyxylulose-5-phosphate synthase (SCO 6768)	Pseudouridine synthase (SCO 1768)	Dihydrolipoamide succinyltransferase (SCO 2181)	Regulator (SCO 1541)	
DNA polymerase III (SCO 4067)	Sugar kinase (SCO 6260)	DNA repair protein (SCO 1780)	SsrA-binding protein, smpB (SCO 2966)	
Glucosamine-fructose-6-phosphate aminotransferase (SCO 2789)	Transcriptional regulator (SCO 3571)	DNA-binding protein (SCO 4944)	Tellurium resistance protein (SCO 4277)	
Glycerol-3-phosphate dehydrogenase (SCO 5559)	Translation initiation factor (SCO 3014)	DNA-directed RNA polymerase beta subunit (SCO 4654)		

GTP-binding protein, EngA (SCO 1758)	Two-component system response regulator (SCO 3008)	Ferredoxin/ferredoxin-NADP reductase (SCO 0681)
Histidine ammonia-lyase, HutH (SCO 4932)		GntR family transcriptional regulator (SCO 1813)
Molybdopterin biosynthesis-like protein, MoeZ (SCO 5178)		Methylmalonyl-CoA mutase (SCO 6832)

Table S6 – Proteins identified to be pupylated in a stationary stage growing culture.

Pupylation Proteins Identified in Stationary Growth					
Wild-Type			<i>Aprc::apr</i>		
30S Ribosomal protein S4 (SCO 1505)	Carbamoylphosphate synthase (SCO 1483)	Precorrin-4 C11-methyltransferase (SCO 1855)	2-amino-3-ketobutyrate coenzyme A ligase (SCO 6800)	PhoH-like protein (SCO 2532)	
30S Ribosomal protein S8 (SCO 4716)	Deoxyxylulose-5-phosphate synthase (SCO 6768)	Protease (SCO 5838)	Acetolactate synthase (SCO 5512)	Phospholipase C (SCO 6691)	
50S Ribosomal protein L4 (SCO 4703)	DNA gyrase subunit B (SCO 3874)	Protein kinase, pglW (SCO 6626)	Allantoate amidohydrolase (SCO 3072)	Regulatory protein (SCO 3664)	
6-Phosphofructokinase, pfkA3 (SCO 1214)	DNA polymerase I, polA (SCO 2003)	Succinate dehydrogenase flavoprotein subunit (SCO 4856)	AraC family transcription regulator, adpA (SCO 2792)	TetR transcriptional regulator (SCO 4907)	
Allantoate amidohydrolase (SCO 3072)	Folylpolyglutamate synthase (SCO 2614)	Succinate dehydrogenase iron-sulfur subunit (SCO 4855)	Glucarate dehydratase (SCO 2542)	Transcription elongation factor, NusA (SCO 5704)	
Arginyl-tRNA synthetase (SCO 3304)	Glucarate dehydratase (SCO 2542)	Tellurium resistance protein (SCO 4277)	Glucose-6-phosphate 1-dehydrogenase (SCO 6661)	Transcriptional regulator (SCO 3571)	
ATP-dependent helicase (SCO 4092)	Isocitrate dehydrogenase (SCO 7000)	TetR transcriptional regulator (SCO 4907)	Isocitrate dehydrogenase (SCO 7000)	Translation initiation factor IF-1 (SCO 4725)	
ATPase AAA (SCO 1648)	NADH dehydrogenase, NuoB (SCO 4563)	Transcription termination factor Rho (SCO 5357)	Nitrate reductase, NarG2 (SCO 0216)		
Bifunctional purine biosynthesis protein (SCO 4814)	Penicillin acylase (SCO 1694)	Transcriptional regulator (SCO 3571)	Oxidoreductase (SCO 7525)		
Branched-chain alpha-keto acid dehydrogenase E1 subunit alpha (SCO 3817)	PhoH-like protein (SCO 2532)		Phenylacetate-CoA ligase (SCO 7469)		

Scanning Electron Microscopy

Streptomyces coelicolor strains to be imaged were plated as lawns on SFM identical to above in the phenotypic analysis section. After growth for 72 hrs, spores were adhered to double-sided tape and subsequently mounted on a microscopy stub. These stubs were then incubated for 48 hrs in the presence of a dehydrating agent (Drierite). After desiccation, the spores were coated with Au by low vacuum sputter coating. The spores were then imaged on a Hitachi 2700 Scanning Electron Microscope equipped with a lanthanum hexaboride gun. Images were collected and analyzed with a Quartz PCI digital imaging system. The microscope was set to a BC of 8, a WD of 15mm, and a KV of 8. The images were collected for 80 seconds with 1.5 K mag, 6 K mag, and 15 K mag, for collection of 20 μm , 5 μm , and 2 μm respectively.

Figure S7: SEM images of *S. coelicolor* *Δpaf::apr* at 20 μm .

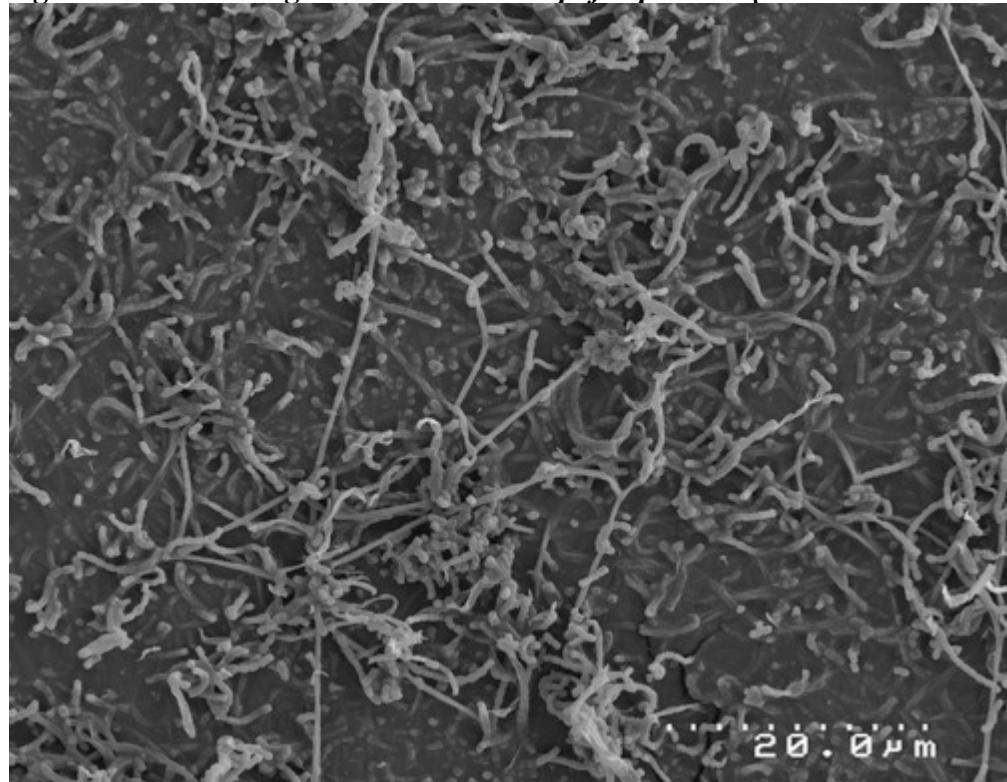


Figure S8: SEM images of *S. coelicolor* *Δpaf::apr* at 5 μm .

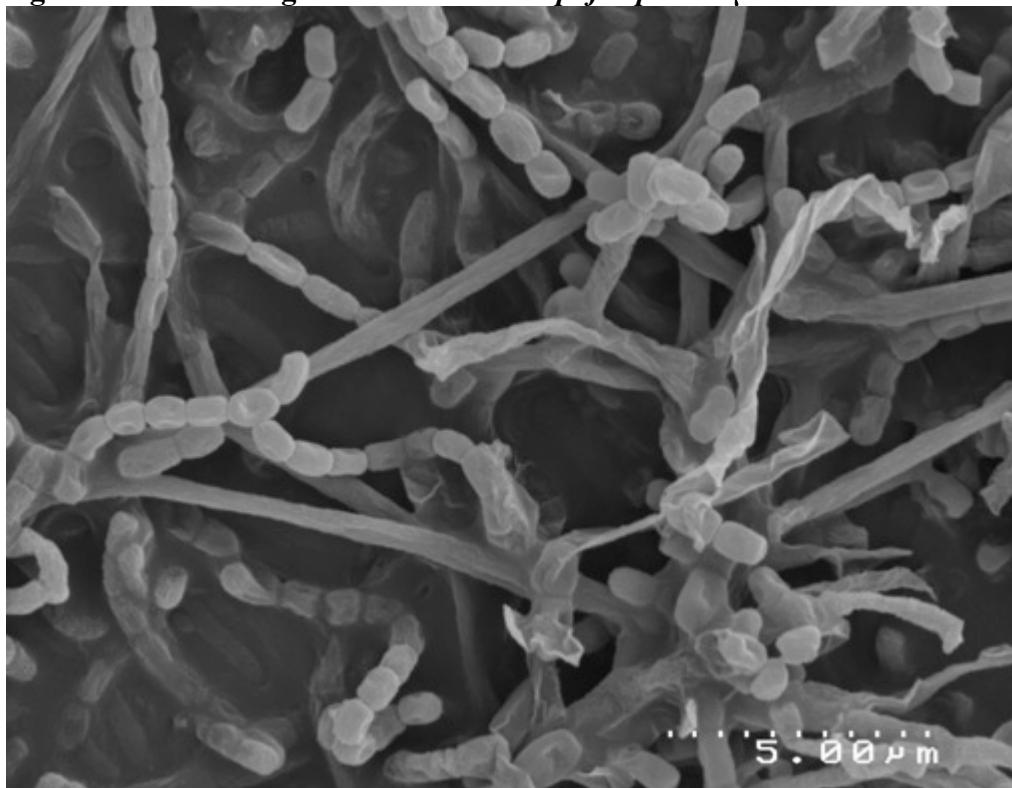


Figure S9: SEM images of *S. coelicolor* *Δpaf::apr* at 2 μm .

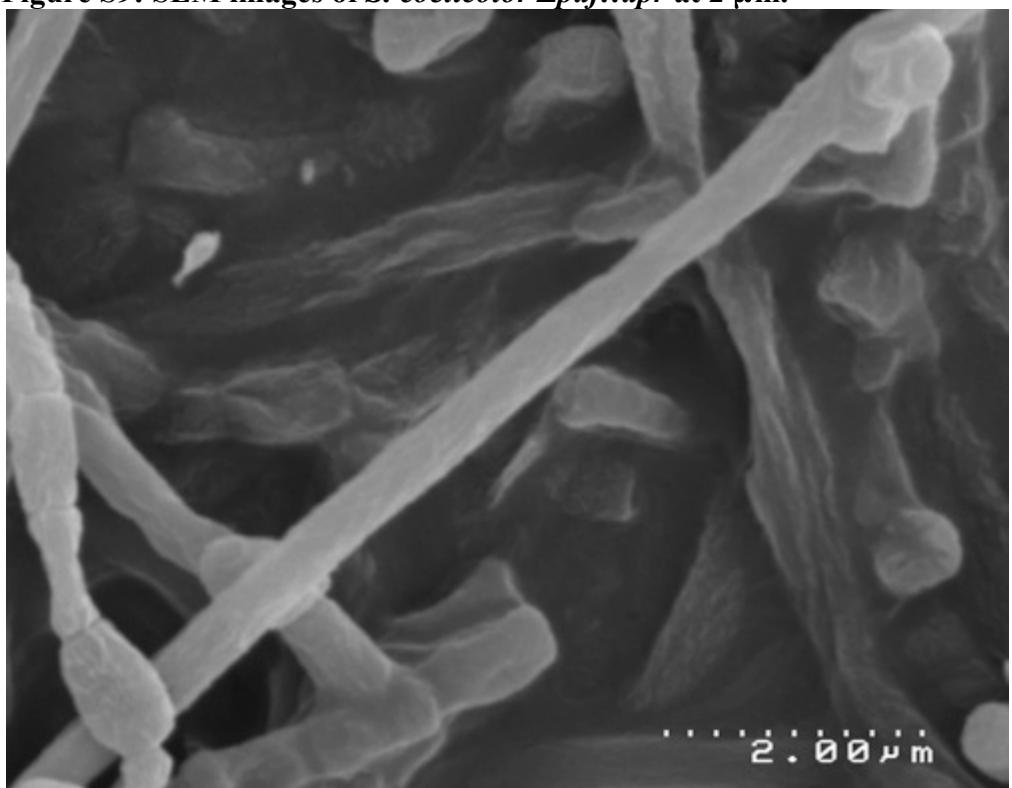


Figure S10: SEM image of *S. coelicolor* M145 WT at 20 μm .

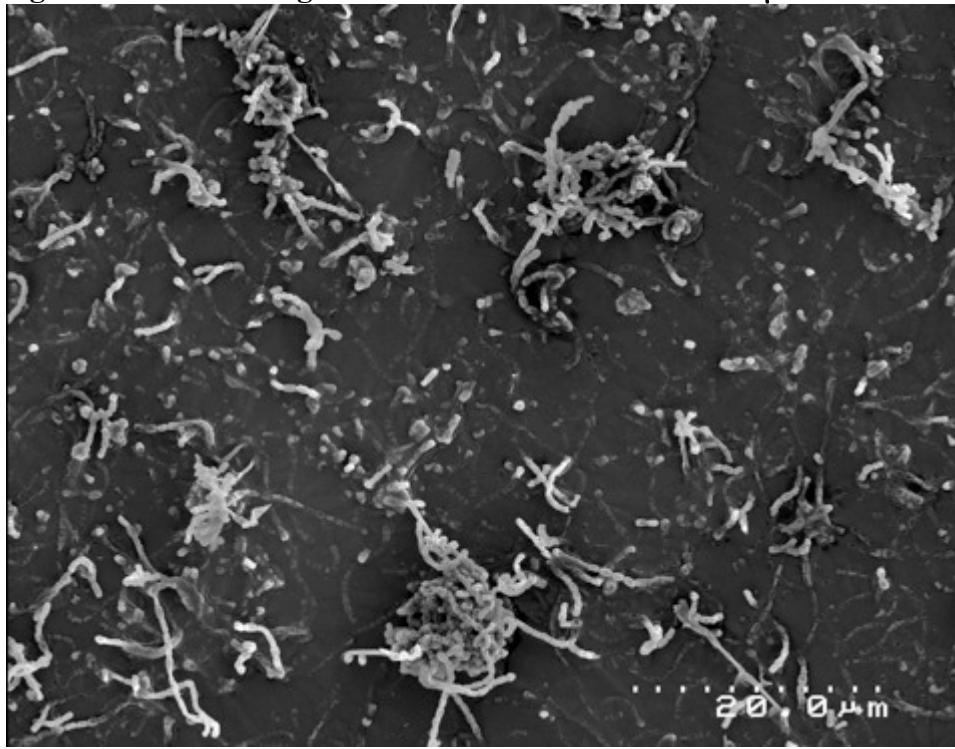


Figure S11: SEM images of *S. coelicolor* M145 WT at 5 μm .

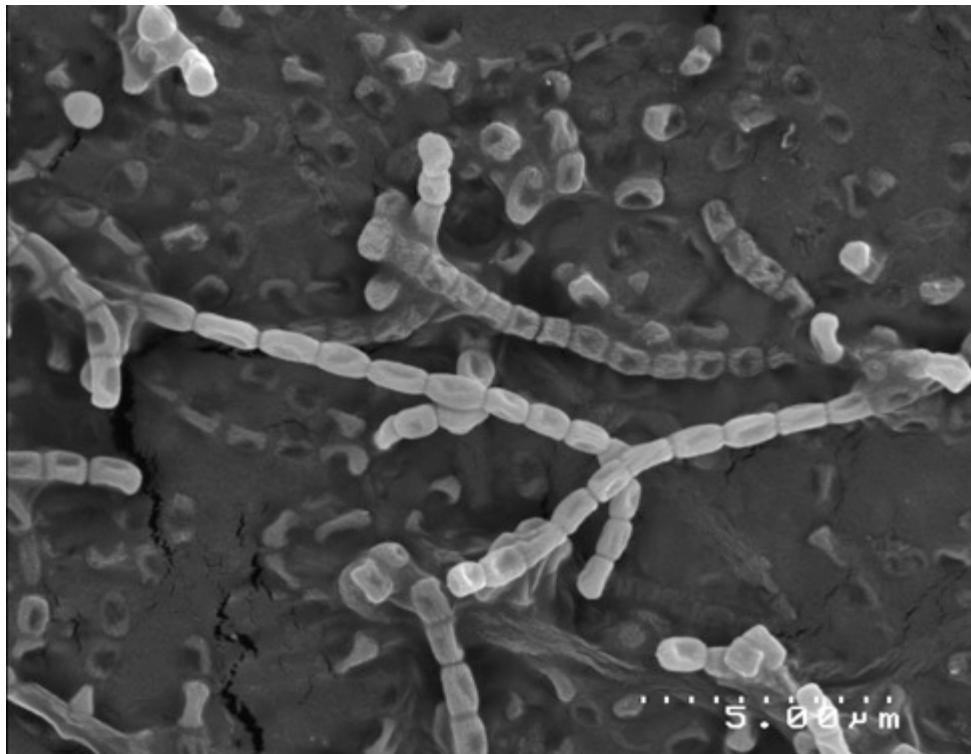


Figure S12: SEM image of *S. coelicolor* M145 WT at 2 μm .



Figure S13: SEM image of *S. coelicolor* ΔpafA with pafA overexpression at 20 μm .

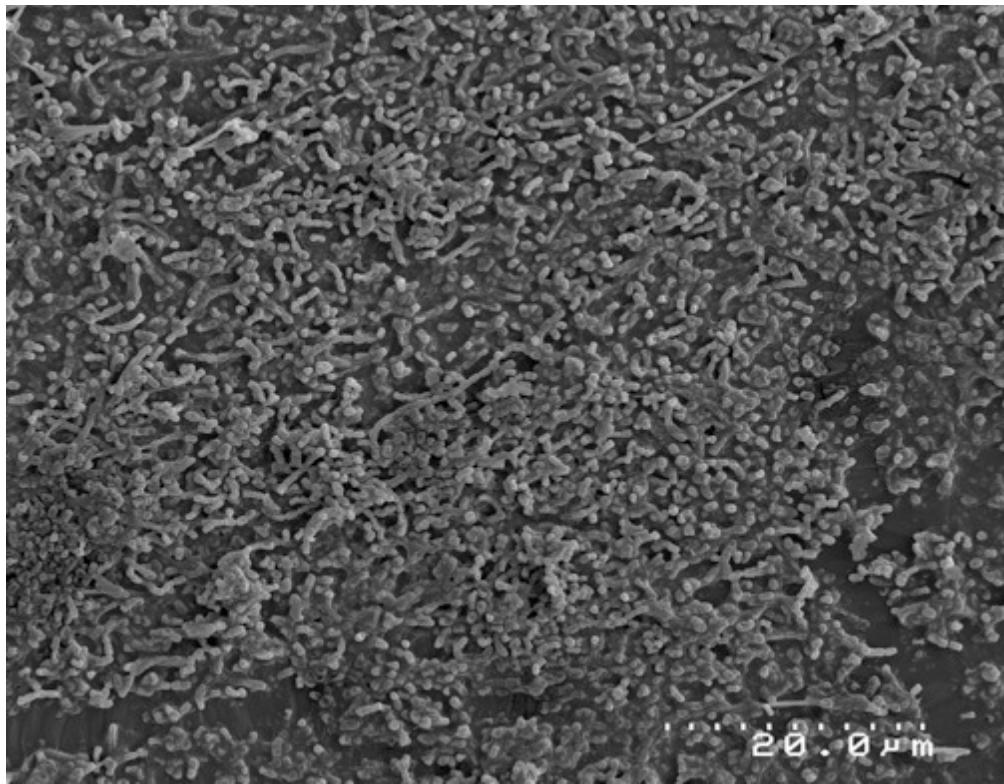


Figure S14: SEM image of *S. coelicolor* Δ pafA with pafA overexpression at 5 μ m.



Figure S15: SEM image of *S. coelicolor* $\Delta pafA$ with *pafA* overexpression at 2 μ m.



Raw Data from Proteomic Analyses

Early Exponential

MS data file: Δpcr: Early Exponential (1).raw
 Instrument type: ESI-FTICR
 Search engine: Mascot
 Parameter file: NCBI-Scoelicolor-FT-alkyl-oxid-tight-HCD.par
 Search database: Scoelicolor_A32_20130406.fasta (16740 entries)
 Enzyme specificity: Trypsin (2 missed cleavages allowed)
 MS mass tolerance: 7 ppm; MS/MS tolerance 20 mmu
 Fixed modifications: Carbamidomethyl (C)
 Var. modifications: [1] Oxidation (M); [2] pupylation (K)
 Number of spectra: 33280
 Input PSMs: 26 'Target'; 3 'Decoy'; 11.5% FDR
 Output PSMs: 26 (31 spectra were assigned to these unique PSMs.)
 Output Proteins: 24 in 24 Protein Groups

<i>Gr p Nr.</i>	<i>Accession Number</i>	<i>Protein Name</i>	<i>Protein Score</i>	<i>Unique PSMs</i>	<i>PSM Serial Nrs.</i>
1	21221001 ref NP_626780.1	glucarate dehydratase [Streptomyces coelicolor A3(2)]	18.17	1	2
2	21222282 ref NP_628061.1	DNA gyrase subunit B [Streptomyces coelicolor A3(2)]	12.97	1	26
3	21224335 ref NP_630114.1	aconitate hydratase [Streptomyces coelicolor A3(2)]	8.00	1	11
4	21224716 ref NP_630495.1	Clp protease ATP binding subunit [Streptomyces coelicolor A3(2)]	6.91	1	17
5	32141309 ref NP_733709.1	hypothetical protein SCO6627, partial [Streptomyces coelicolor A3(2)]	5.23	1	18
6	Q7Z3Z0	Tax_Id=9606 Gene_Symbol=KRT25 Keratin, type I cytoskeletal 25	4.66	1	24
7	32141270 ref NP_733671.1	translation initiation factor IF-2 [Streptomyces coelicolor A3(2)]	4.22	1	20
8	21223834 ref NP_629613.1	oligopeptide-binding lipoprotein [Streptomyces coelicolor A3(2)]	3.65	2	1 4
9	21222550 ref NP_628329.1	5~-nucleotidase [Streptomyces coelicolor A3(2)]	3.18	1	6

10	21223041 ref NP_628820.1	30S ribosomal protein S7 [Streptomyces coelicolor A3(2)]	2.89	2	8 25
11	21220785 ref NP_626564.1	methyltransferase [Streptomyces coelicolor A3(2)]	2.11	1	5
12	21223186 ref NP_628965.1	succinyl-CoA synthetase subunit beta [Streptomyces coelicolor A3(2)]	1.91	1	23
13	P08779	Tax_Id=9606 Gene_Symbol=KRT16 Keratin, type I cytoskeletal 16	1.44	1	9
14	21220260 ref NP_626039.1	pseudouridine synthase [Streptomyces coelicolor A3(2)]	1.43	1	15
15	21221781 ref NP_627560.1	DNA integrity scanning protein DisA [Streptomyces coelicolor A3(2)]	1.39	1	14
16	21222670 ref NP_628449.1	tellurium resistance protein [Streptomyces coelicolor A3(2)]	1.14	1	21
17	21223756 ref NP_629535.1	cellulose-binding protein [Streptomyces coelicolor A3(2)]	0.99	1	10
18	21222311 ref NP_628090.1	hypothetical protein SCO3904 [Streptomyces coelicolor A3(2)]	0.67	1	3
19	21223817 ref NP_629596.1	enoyl-CoA hydratase [Streptomyces coelicolor A3(2)]	0.42	1	12
20	21224924 ref NP_630703.1	protein kinase [Streptomyces coelicolor A3(2)]	0.37	1	13
21	161353681 ref NP_625871.2	phenylalanyl-tRNA synthetase subunit alpha [Streptomyces coelicolor A3(2)]	0.13	1	19
22	21225061 ref NP_630840.1	1-deoxy-D-xylulose-5-phosphate synthase [Streptomyces coelicolor A3(2)]	0.06	1	16
23	21224363 ref NP_630142.1	uroporphyrinogen decarboxylase [Streptomyces coelicolor A3(2)]	0.01	1	7
24	21220520 ref NP_626299.1	indole-3-glycerol-phosphate synthase [Streptomyces coelicolor A3(2)]	0.01	1	22

Group Nr. By the rule of parsimony, we have gathered all proteins sharing the same identified peptides into a single group.

Accession Nr. The accession number from the searched database (DB).

Protein Name The protein name in the DB.

Protein Score Sum of the contributing peptide scores.

NOTE: This score can only be used to support the identification of **one** protein per group.

Unique PSMs. The number of unique peptide-spectrum matches that contribute to the protein assignment.

PSM Serial Nrs. Sequential number of assigned peptide (in the following table.)

Other Grp. If the protein is assigned to another group, that (those) group number(s).

Score (Other) Protein score (as above) for this protein in other group(s).

Assigned Peptides										
#	Sequence	PTM Site	Nr. Scan s	Masco t Score	Expec tation	Isola ted Mass	Delta Mass	Char ge State	Match ed Ions	Scan Nr.
1	K.KGNVEKAK.E	0.00000200.0	1	0.070	6	558.80	1.3	2	'2/14	5197
2	R.LAFDGGK.V	0.0000002.0	2	18.170	0.059	475.73	1.8	2	'4/12	8650
3	K.KGIQDPDVK.R	0.000000002.0	1	0.670	3	621.82	0.2	2	'3/16	8163
4	K.ACNPNGFKTTIA VR.N	0.000000002000 000.0	1	3.580	1.9	960.48	1.8	2	'4/28	13234
5	R.AYHKLLVWDIMKK PLATR.V	0.000200000012 200000.0	1	2.110	2.7	732.88	1.9	4	'3/34	30150
6	R.VTEVQPDGTTK.T	0.00000000002.0	1	3.180	1.7	709.34	1.9	2	'3/20	13353
7	R.ELGATPLIGFAGAP FTLASYLVEGGPSRN HEHTKA	0.000000000000 0000000000000000 00000002.0	1	0.010	3.1	1260.97	0.7	3	'3/66	28714
8	M.PRKGPAK.R	0.00200000.0	1	0.010	1.2	547.31	1.4	2	'2/14	6568
9	K.EELAYLRKNHEEE MLALR.G	0.000000020000 000000.0	1	1.440	3.5	829.75	2.4	3	'3/34	22973
10	R.IVEKAKGDASQLR.S	0.000002000000 0.0	1	0.990	5.3	553.30	0.8	3	'3/24	11902
11	K.AVEKGLTR.K	0.00020000.0	1	8.000	0.97	558.80	1.3	2	'3/14	5197
12	K.VFAAGADIKEMQV MDHAAMIARS	0.000000002000 0000001000.0	1	0.420	2.7	1317.63	2.1	2	'2/42	37217
13	R.FPELKPMRDAWR.K	0.000020100000.0	2	0.370	3.3	602.30	3.1	3	'3/22	17786
14	R.TADRVSKQVGFPV VSVSQSMR.L	0.000000200000 000000010.0	1	1.390	3.7	846.43	0.9	3	'5/40	19190
15	R.VVEQTGKNYLVEV TLHEGRK.H	0.000000200000 00000002.0	1	1.430	5	929.14	2.2	3	'3/38	37307

16	K.LLTGRQDFSKLR.S	0.000000000200.0	1	0.060	3.7	559.64	1.1	3	'2/22	11270
17	R.IEKDAALAR.R	0.002000000.0	1	6.910	1.2	615.33	0.7	2	'3/16	8592
18	K.AVEADLGKQVK.A	0.00000002000.0	1	5.230	2.1	700.87	3.5	2	'5/20	14753
19	-MKPEEIERMR.D	0.12000000000.0	1	0.130	2.2	789.37	5.3	2	'3/18	9778
20	K.RNTKAR.L	0.000200.0	3	4.220	2.5	494.77	4.1	2	'3/10	17645
21	-MAVSLSKGGNVSLT.K.E	0.100000200000.000.0	2	1.140	4.1	584.31	0.8	3	'3/28	3781
22	K.VIGVNARNLKT	0.0000000002.0	1	0.010	3.8	663.88	3.9	2	'2/18	16425
23	K.SVVKAQVKVGGR.G	0.000200000000.0	1	1.910	3.2	735.92	4.1	2	'2/22	11070
24	R.SKILTTTR.L	0.0200000.0	1	4.660	1.1	531.30	2.1	2	'2/12	6526
25	K.VLLNGKRS	0.0000020.0	1	2.880	3.1	521.80	0.7	2	'3/12	5906
26	R.NAKDVR.F	0.002000.0	1	12.970	0.25	473.24	2.3	2	'3/10	11304
			31							

Serial (sequential) number for peptide.

Sequence Assigned peptide sequence. Periods (".") delimit the sequence for internal peptides.

PTM Site Location of the post-translational modification (PTM) in the peptide.

Modification codes: [1] Oxidation (M); [2] Pupylation (K)

Nr. Scans The number of MS/MS scans that were matched to this peptide.

Mascot Score Score given to this peptide/spectrum match by Mascot.

Expectation The number of matches with equal or better scores that are expected to occur by chance alone.

Isolated Mass "Mass" in the Orbitrap analyzer.

Delta Mass Difference between the observed and theoretical masses, in ppm.

Charge State Inferred ionic state of the peptide.

Matched Ions Number of matched MS/MS ions, as reported by Mascot. NOTE: Temporarily disabled.

Scan Nr. MS/MS scan number in the original Xcalibur RAW file.

MS data file: Δprc Early Exponential (2).raw

Instrument type: ESI-FTICR

Search engine: Mascot
 Parameter file: NCBI-Scoelicolor-FT-alkyl-oxid-tight-HCD.par
 Search database: Scoelicolor_A32_20130406.fasta (16740 entries)
 Enzyme specificity: Trypsin (2 missed cleavages allowed)
 MS mass tolerance: 7 ppm; MS/MS tolerance 20 mmu
 Fixed modifications: Carbamidomethyl (C)
 Var. modifications: [1] Oxidation (M); [2] pupylation (K)
 Number of spectra: 34542
 Input PSMs: 36 'Target'; 3 'Decoy'; 8.3% FDR
 Output PSMs: 36 (70 spectra were assigned to these unique PSMs.)
 Output Proteins: 32 in 32 Protein Groups

<i>Gr p N r.</i>	<i>Accessi on Numbe r.</i>	<i>Protein Name</i>	<i>Protein Score</i>	<i>Unique PSMs</i>	<i>PSM Serial Nrs.</i>
1	212215 13 ref NP_627 292.1	allantoate amidohydrolase [Streptomyces coelicolor A3(2)]	11.01	1	36
2	212236 30 ref NP_629 409.1	hypothetical protein SC05263 [Streptomyces coelicolor A3(2)]	8.53	1	11
3	212202 60 ref NP_626 039.1	pseudouridine synthase [Streptomyces coelicolor A3(2)]	8.25	2	3 21
4	212220 78 ref NP_627 857.1	regulatory protein [Streptomyces coelicolor A3(2)]	7.57	1	15
5	212219 62 ref NP_627 741.1	DNA topoisomerase I [Streptomyces coelicolor A3(2)]	6.78	2	9 10
6	212219 89 ref NP_627 768.1	transcriptional regulator [Streptomyces coelicolor A3(2)]	5.14	1	5
7	212237 57 ref NP_629 536.1	large Ala/Glu-rich protein [Streptomyces coelicolor A3(2)]	4.71	2	8 26
8	321412 13 ref NP_733 614.1	molecular chaperone DnaK [Streptomyces coelicolor A3(2)]	4.62	1	14

9	212226 89 refl NP_628 468.1	chaperonin GroEL [Streptomyces coelicolor A3(2)]	4.33	1	6
10	212241 87 refl NP_629 966.1	hypothetical protein SC05843 [Streptomyces coelicolor A3(2)]	3.57	1	31
11	212206 98 refl NP_626 477.1	bifunctional alpha-amylase/dextrinase [Streptomyces coelicolor A3(2)]	3.46	1	20
12	212258 36 refl NP_631 615.1	oxidoreductase [Streptomyces coelicolor A3(2)]	3.16	1	27
13	212207 48 refl NP_626 527.1	hypothetical protein SC02279 [Streptomyces coelicolor A3(2)]	3.05	1	34
14	212205 20 refl NP_626 299.1	indole-3-glycerol-phosphate synthase [Streptomyces coelicolor A3(2)]	3.03	1	32
15	321413 09 refl NP_733 709.1	hypothetical protein SC06627, partial [Streptomyces coelicolor A3(2)]	2.76	1	28
16	212249 24 refl NP_630 703.1	protein kinase [Streptomyces coelicolor A3(2)]	2.42	1	19
17	212224 91 refl NP_628 270.1	valine dehydrogenase [Streptomyces coelicolor A3(2)]	2.21	1	16
18	212250 01 refl NP_630 780.1	ATP-dependent DNA ligase [Streptomyces coelicolor A3(2)]	2.01	2	1 33
19	212224 98 refl NP_628 277.1	ATP-dependent RNA helicase [Streptomyces coelicolor A3(2)]	1.98	1	30
20	212244 94 refl NP_630 273.1	regulatory protein [Streptomyces coelicolor A3(2)]	1.51	1	18
21	212203 04 refl NP_626	enoyl-ACP reductase [Streptomyces coelicolor A3(2)]	1.27	1	25

	083.1				
22	212216 22 ref NP_627 401.1	hypothetical protein SCO3187 [Streptomyces coelicolor A3(2)]	1.23	1	17
23	212249 04 ref NP_630 683.1	hypothetical protein SCO6606 [Streptomyces coelicolor A3(2)]	0.97	1	23
24	212205 69 ref NP_626 348.1	UDP-N-acetylmuramoylalanyl-D-glutamate--2,6-diaminopimelate ligase [Streptomyces coelicolor A3(2)]	0.74	1	12
25	161353 681 ref NP_625 871.2	phenylalanyl-tRNA synthetase subunit alpha [Streptomyces coelicolor A3(2)]	0.74	1	22
26	212248 19 ref NP_630 598.1	uvrA-like protein [Streptomyces coelicolor A3(2)]	0.66	1	2
27	212244 31 ref NP_630 210.1	nitrite/sulfite reductase [Streptomyces coelicolor A3(2)]	0.57	1	24
28	212214 48 ref NP_627 227.1	preprotein translocase subunit SecA [Streptomyces coelicolor A3(2)]	0.55	1	7
29	212207 85 ref NP_626 564.1	methyltransferase [Streptomyces coelicolor A3(2)]	0.50	1	4
30	212200 97 ref NP_625 876.1	translation initiation factor IF-3 [Streptomyces coelicolor A3(2)]	0.49	1	13
31	212203 40 ref NP_626 119.1	cob(I)yrinic acid a,c-diamide adenosyltransferase [Streptomyces coelicolor A3(2)]	0.46	1	35
32	313405 47 ref NP_733 545.1	hypothetical protein SCO1793, partial [Streptomyces coelicolor A3(2)]	0.36	1	29

Group Nr. By the rule of parsimony, we have gathered all proteins sharing the same identified peptides into a single group.

Accession Nr. The accession number from the searched database (DB).

Protein Name The protein name in the DB.

Protein Score Sum of the contributing peptide scores.

NOTE: This score can only be used to support the identification of **one** protein per group.

Unique PSMs. The number of unique peptide-spectrum matches that contribute to the protein assignment.

PSM Serial Nrs. Sequential number of assigned peptide (in the following table.)

Other Grp. If the protein is assigned to another group, that (those) group number(s).

Score (Other) Protein score (as above) for this protein in other group(s).

Assigned Peptides										
#	Sequence	PTM Site	Nr. Scans	Mascot Score	Expectation	Isolated Mass	Delta Mass	Charge State	Matched Ions	Scan Nr.
1	R.GLLQHVGVSAAFT MK.R	0.0000000000000002 .0	1	0.460	6	901.4 6	5.0	2	'4/28	18569
2	K.SFLSKDK.E	0.0000202.0	1	0.660	2.7	655.8 2	6.9	2	'2/12	6900
3	R.TAFGPITLGDQKSG WLRR.L	0.000000000002000 000.0	1	2.410	3.1	749.3 9	5.4	3	'2/34	4162
4	R.AYHKLLVWDIMKK PLATR.V	0.000200000012200 000.0	2	0.500	3.7	732.8 8	1.0	4	'3/34	2980
5	R.ETVNKALADFAQR GWLR.L	0.000020000000000 00.0	7	5.140	2.2	555.2 9	0.9	4	'4/32	28598
6	-MAKIIAFDEEARR.G	0.1020000000000.0	1	4.330	2	603.6 4	5.3	3	'3/24	26984
7	K.LMRAGEGKILR.K	0.00000002000.0	1	0.550	6.1	496.2 7	6.1	3	'3/20	34195
8	R.IVAEAAEKART	0.0000000200.0	1	3.420	3.6	650.8 4	5.6	2	'3/18	33446
9	K.NAVKPR.T	0.000200.0	1	5.930	0.75	464.2 5	0.8	2	'2/10	6328
10	K.KVMPRLSAGR.V	0.2010000000.0	1	0.850	6	687.3 7	0.7	2	'3/18	11044
11	R.GAKEVLEKA	0.00200000.0	1	8.530	0.93	558.8 0	2.9	2	'5/14	6076
12	R.IKSERTTPEATDLQ ALFAVMR.E	0.020000000000000 000010.0	1	0.740	3	879.4 5	0.2	3	'3/40	17028
13	K.FKYESAMKAR.E	0.0200001000.0	1	0.490	2.7	745.3 6	1.6	2	'2/18	7449
14	K.LKGEDTAEIR.T	0.0200000000.0	1	4.620	1.5	687.8 4	5.1	2	'2/18	10172
15	R.DKTLTERGVRI	0.0200000000.0	1	7.570	1.2	473.2 5	2.8	3	'3/18	13662

16	R.TVGIAGVGK.V	0.000000002.0	1	2.210	7	522.7 9	4.1	2	'5/16	10895
17	K.KVFSAVGIVFKGSG FYR.N	0.200000000020000 00.0	1	1.230	3.1	1174. 60	4.6	2	'2/32	31147
18	R.ALDDTDALGLK.L	0.00000000002.0	1	1.510	4.9	458.2 5	2.6	3	'2/20	16762
19	R.FPELKPMRDAWR. K	0.000020100000.0	2	2.420	1.9	602.3 0	2.8	3	'3/22	20750
20	R.VGAAAGTGYRLHP VQAAGADAVVK.E	0.000000000000000 000000002.0	1	3.460	2	1261. 66	0.7	2	'3/46	29987
21	R.VVEQTGKNYLVEV TLHEGRK.H	0.0000020000000 00002.0	1	5.840	1.8	929.1 4	2.2	3	'5/38	35423
22	-MKPEEIER.M	0.02000000.0	1	0.740	2.7	637.8 1	6.4	2	'3/14	15469
23	R.REDAAAVYNK.A	0.0000000002.0	1	0.970	2.6	690.3 3	0.1	2	'3/18	8137
24	-MAATPPKPAAATPR. R	0.0000002000000. 0	1	0.570	4.6	811.9 2	4.5	2	'3/26	15284
25	R.YMARDLGKQNI.R.C	0.010000020000.0	1	1.270	3.8	575.2 9	6.7	3	'2/22	35860
26	R.MSEAEELRKAQA EAEK.V	0.000000000200000 00.0	1	1.290	2.6	1067. 51	2.2	2	'3/32	7154
27	R.AGLTALLGPDKVL WK.V	0.000000000000002 .0	1	3.160	1.2	609.0 1	3.4	3	'4/28	20386
28	K.AVEADLGKQVK.A	0.00000000002.0	1	2.760	3.7	700.8 7	3.5	2	'6/20	17771
29	R.FKSADMER.G	0.02000000.0	1	0.360	1.7	613.7 7	5.5	2	'2/14	6123
30	R.DAGAKADALHGG MTQGARTR.T	0.000020000000000 00000.0	1	1.980	1.8	1114. 03	4.7	2	'2/38	23809
31	-MAKTSTTTQGLR.A	0.102000000000.0	1	3.570	1.8	777.3 8	3.9	2	'2/22	10844
32	K.VIGVNARNLK.T	0.0000000002.0	1	3.030	1.7	663.8 7	5.9	2	'2/18	19244
33	M.DLPVMPPVKPML AK.S	0.00001000200002. 0	4	1.550	2.8	1019. 53	6.2	2	'3/26	34082
34	R.RPKEAAGDGGR.E	0.00200000000.0	1	3.050	0.94	678.8 3	6.4	2	'2/20	4527
35	R.EGW_EQVKR.D	0.00000020.0	1	0.460	2.9	637.8 1	0.2	2	'3/14	15469
36	R.REAQLAGAVATFG K.I	0.00000000000002. 0	24	11.01 0	0.43	831.4 4	2.6	2	'3/26	3592
			70							

#

Serial (sequential) number for peptide.

Sequence Assigned peptide sequence. Periods (".") delimit the sequence for internal peptides.
PTM Site Location of the post-translational modification (PTM) in the peptide.
 Modification codes: [1] Oxidation (M); [2] pupylation (K)
Nr. Scans The number of MS/MS scans that were matched to this peptide.
Mascot Score Score given to this peptide/spectrum match by Mascot.
Expectation The number of matches with equal or better scores that are expected to occur by chance alone.
Isolated Mass "Mass" in the Orbitrap analyzer.
Delta Mass Difference between the observed and theoretical masses, in ppm.
Charge State Inferred ionic state of the peptide.
Matched Ions Number of matched MS/MS ions, as reported by Mascot. NOTE:
 Temporarily disabled.
Scan Nr. MS/MS scan number in the original Xcalibur RAW file.

MS data file: WT Early Exponential (1).raw
 Instrument type: ESI-FTICR
 Search engine: Mascot
 Parameter file: NCBI-Scoelicolor-FT-alkyl-oxid-tight-HCD.par
 Search database: Scoelicolor_A32_20130406.fasta (16740 entries)
 Enzyme specificity: Trypsin (2 missed cleavages allowed)
 MS mass tolerance: 7 ppm; MS/MS tolerance 20 mmu
 Fixed modifications: Carbamidomethyl (C)
 Var. modifications: [1] Oxidation (M); [2] pupylation (K)
 Number of spectra: 29826
 Input PSMs: 31 'Target'; 2 'Decoy'; 6.5% FDR
 Output PSMs: 31 (34 spectra were assigned to these unique PSMs.)
 Output Proteins: 30 in 30 Protein Groups

<i>Gr p N r.</i>	<i>Accession Number</i>	<i>Protein Name</i>	<i>Protein Score</i>	<i>Unique PSMs</i>	<i>PSM Serial Nrs.</i>
1	32141309 ref NP_73 3709.1	hypothetical protein SCO6627, partial [Streptomyces coelicolor A3(2)]	10.79	1	27
2	21220992 ref NP_62 6771.1	PhoH-like protein [Streptomyces coelicolor A3(2)]	10.56	1	18
3	21222282 ref NP_62 8061.1	DNA gyrase subunit B [Streptomyces coelicolor A3(2)]	10.24	1	31
4	21223231 ref NP_62 9010.1	succinate dehydrogenase iron-sulfur subunit [Streptomyces coelicolor A3(2)]	6.85	1	28

5	21223482 ref NP_62 9261.1	GTP-binding protein [Streptomyces coelicolor A3(2)]	5.94	1	12
6	21222715 ref NP_62 8494.1	hydrolase [Streptomyces coelicolor A3(2)]	5.34	1	21
7	21223041 ref NP_62 8820.1	30S ribosomal protein S7 [Streptomyces coelicolor A3(2)]	4.99	1	29
8	21224182 ref NP_62 9961.1	protease [Streptomyces coelicolor A3(2)]	4.87	1	30
9	21224335 ref NP_63 0114.1	aconitate hydratase [Streptomyces coelicolor A3(2)]	3.84	1	15
10	21224773 ref NP_63 0552.1	acyl-CoA dehydrogenase [Streptomyces coelicolor A3(2)]	3.13	1	9
11	21223101 ref NP_62 8880.1	50S ribosomal protein L15 [Streptomyces coelicolor A3(2)]	2.88	1	19
12	21223756 ref NP_62 9535.1	cellulose-binding protein [Streptomyces coelicolor A3(2)]	2.53	1	24
13	21222044 ref NP_62 7823.1	adenylosuccinate synthetase [Streptomyces coelicolor A3(2)]	2.37	1	11
14	21222641 ref NP_62 8420.1	hypothetical protein SC04246 [Streptomyces coelicolor A3(2)]	2.25	1	14
15	21222543 ref NP_62 8322.1	polyphosphate kinase [Streptomyces coelicolor A3(2)]	1.77	1	4
16	32141192 ref NP_73 3593.1	bifunctional N-acetylglucosamine-1-phosphate uridyltransferase/glucosamine-1-phosphate acetyltransferase [Streptomyces coelicolor A3(2)]	1.68	1	20
17	21220009 ref NP_62 5788.1	histidyl-tRNA synthetase [Streptomyces coelicolor A3(2)]	1.52	1	5
18	21221297 ref NP_62 7076.1	oxidoreductase [Streptomyces coelicolor A3(2)]	1.41	1	7
19	32141270 ref NP_73 3671.1	translation initiation factor IF-2 [Streptomyces coelicolor A3(2)]	1.23	1	26
20	21221779 ref NP_62 7558.1	hypothetical protein SC03349 [Streptomyces coelicolor A3(2)]	1.07	1	22
21	21224924	protein kinase [Streptomyces coelicolor]	0.99	1	17

	ref NP_63 0703.1	A3(2)]			
22	21222311 ref NP_62 8090.1	hypothetical protein SC03904 [Streptomyces coelicolor A3(2)]	0.91	1	6
23	21222206 ref NP_62 7985.1	aspartyl-tRNA synthetase [Streptomyces coelicolor A3(2)]	0.70	1	1
24	21224431 ref NP_63 0210.1	nitrite/sulfite reductase [Streptomyces coelicolor A3(2)]	0.67	1	23
25	21224123 ref NP_62 9902.1	glutamate uptake system ATP-binding protein [Streptomyces coelicolor A3(2)]	0.65	2	28
26	32141213 ref NP_73 3614.1	molecular chaperone DnaK [Streptomyces coelicolor A3(2)]	0.38	1	13
27	21221546 ref NP_62 7325.1	lipoprotein [Streptomyces coelicolor A3(2)]	0.31	1	16
28	21222139 ref NP_62 7918.1	stress response protein [Streptomyces coelicolor A3(2)]	0.25	1	10
29	21223106 ref NP_62 8885.1	30S ribosomal protein S13 [Streptomyces coelicolor A3(2)]	0.07	1	3
30	21223982 ref NP_62 9761.1	ribosome recycling factor [Streptomyces coelicolor A3(2)]	0.03	1	25

Group Nr. By the rule of parsimony, we have gathered all proteins sharing the same identified peptides into a single group.

Accession Nr. The accession number from the searched database (DB).

Protein Name The protein name in the DB.

Protein Score Sum of the contributing peptide scores.

NOTE: This score can only be used to support the identification of **one** protein per group.

Unique PSMs. The number of unique peptide-spectrum matches that contribute to the protein assignment.

PSM Serial Nrs. Sequential number of assigned peptide (in the following table.)

Other Grp. If the protein is assigned to another group, that (those) group number(s).

Score (Other) Protein score (as above) for this protein in other group(s).

Assigned Peptides

#	Sequence	PTM Site	Nr. Scans	Mascot Score	Expectation	Isolated Mass	Delta Mass	Charge State	Matched Ions	Scan Nr.
1	K.YGSDKPDLRA	0.000020000.0	1	0.700	3.5	647.31	4.5	2	'4/16	15675
2	R.ALAMDPKVMLFDE PTSALDPEMINEVLE VMK.Q	0.000000001000000 000000000000000002. 0	1	0.240	2.6	1245.94	4.8	3	'3/60	14780
3	R.AIAGKK.K	0.000022.0	1	0.070	7.2	537.28	2.7	2	'2/10	7098
4	R.RYSHVGTGNYHPK TAR.L	0.000000000000200 0.0	1	1.770	3.3	1044.01	1.8	2	'2/30	5304
5	K.AAMKAANRSGAR. Y	0.001200000000.0	1	1.520	3.6	731.86	3.6	2	'2/22	6361
6	K.KGIQDPDVK.R	0.000000002.0	1	0.910	2.8	621.82	0.2	2	'3/16	8478
7	R.ALEAGLPVVVDKP VAGTAAEAR.A	0.000000000002000 0000000.0	1	1.410	1.8	793.10	5.6	3	'4/42	21510
8	K.KAEEKARA.A	0.0000200.0	1	0.410	6.6	537.78	0.9	2	'2/12	4817
9	K.IDKMGYKGVDTTE LIMDGLR.I	0.002100200000000 10000.0	1	3.130	1.7	1387.16	3.9	2	'2/38	5528
10	K.KGSSFQKAR.N	0.000000200.0	1	0.250	4.3	417.88	4.2	3	'2/16	8276
11	R.GIGPTYADKINR.V	0.000000002000.0	1	2.370	2.9	774.39	5.5	2	'3/22	12137
12	K.EVEGKTYEPVER.M	0.000020000000.0	1	5.940	0.75	839.90	0.5	2	'4/22	28191
13	K.LKGEDTAEIR.T	0.0200000000.0	1	0.380	4.1	687.84	5.8	2	'2/18	8519
14	K.MIMYLDSKGKFR.F	0.000000000200.0	1	2.250	1.9	866.43	1.7	2	'3/22	7785
15	K.AVEKGLTR.K	0.00020000.0	1	3.840	2.4	558.80	1.8	2	'3/14	4866
16	K.ASEVQIDHVVPPLSY SWQMGSRWPNK R.E	0.000000000000000 00000000000020.0	1	0.310	3	883.18	1.8	4	'2/54	16895
17	R.FPELKPMRDAWR. K	0.000020100000.0	2	0.990	3.2	602.30	1.6	3	'3/22	19115
18	K.AVQALQSK.Q	0.00000002.0	2	10.560	0.71	544.29	4.0	2	'3/14	8310
19	R.KNSLVK.V	0.200002.0	1	2.880	3	587.81	1.0	2	'3/10	16077
20	K.RPGSAAKAAEAV SR.E	0.0000002000000 .0	1	1.680	3.4	421.97	6.4	4	'3/28	8049
21	R.AVVVTAKYEPNAK. L	0.0000002000002.0	1	5.340	1.7	625.99	4.9	3	'4/24	13485

22	K.KAKDEK.S	0.002000.0	1	1.070	5.3	481.2 5	5.6	2	'2/10	3420
23	-MAATPPKPAAATPR.R	0.00000020000000.	1	0.670	5.4	811.9 2	0.5	2	'3/26	13274
24	K.AKGDASQLR.S	0.020000000.0	1	2.530	3.7	594.8 0	3.4	2	'4/16	6855
25	K.GEDAKVSIR.S	0.000020000.0	1	0.030	6.5	609.3 1	0.6	2	'2/16	5602
26	K.RNTKAR.L	0.000200.0	1	1.230	5.6	494.7 7	1.2	2	'3/10	32725
27	K.AVEADLGKQVK.A	0.0000000002.0	2	10.79 0	0.55	700.8 7	3.8	2	'3/20	15595
28	K.AIAEVKRA.A	0.0000020.0	1	6.850	1.5	515.2 9	3.9	2	'3/12	9523
29	K.VLLNGKRS	0.0000020.0	1	4.990	1.9	521.8 0	2.9	2	'5/12	5674
30	R.EEKGYTYGVRAFG QVLR.S	0.00200000000000 00.0	1	4.870	2	1108. 56	1.5	2	'2/32	14318
31	R.NAKDVR.F	0.002000.0	1	10.24 0	0.49	473.2 4	0.8	2	'3/10	12064
			34							

Serial (sequential) number for peptide.

Sequence Assigned peptide sequence. Periods (".") delimit the sequence for internal peptides.

PTM Site Location of the post-translational modification (PTM) in the peptide.
Modification codes: [1] Oxidation (M); [2] pupylation (K)

Nr. Scans The number of MS/MS scans that were matched to this peptide.

Mascot Score Score given to this peptide/spectrum match by Mascot.

Expectation The number of matches with equal or better scores that are expected to occur by chance alone.

Isolated Mass "Mass" in the Orbitrap analyzer.

Delta Mass Difference between the observed and theoretical masses, in ppm.

Charge State Inferred ionic state of the peptide.

Matched Ions Number of matched MS/MS ions, as reported by Mascot. NOTE:
Temporarily disabled.

Scan Nr. MS/MS scan number in the original Xcalibur RAW file.

MS data file: WT Early Exponential (2).raw

Instrument type: ESI-FTICR

Search engine: Mascot

Parameter file: NCBI-Scoelicolor-FT-alkyl-oxid-tight-HCD.par

Search database: Scoelicolor_A32_20130406.fasta (16740 entries)
 Enzyme specificity: Trypsin (2 missed cleavages allowed)
 MS mass tolerance: 7 ppm; MS/MS tolerance 20 mmu
 Fixed modifications: Carbamidomethyl (C)
 Var. modifications: [1] Oxidation (M); [2] pupylation (K)
 Number of spectra: 32346
 Input PSMs: 59 'Target'; 3 'Decoy'; 5.1% FDR
 Output PSMs: 59 (76 spectra were assigned to these unique PSMs.)
 Output Proteins: 57 in 56 Protein Groups

<i>Gr p N r.</i>	<i>Accessi on Numbe r.</i>	<i>Protein Name</i>	<i>Protein Score</i>	<i>Unique PSMs</i>	<i>PSM Serial Nrs.</i>
1	212210 01 ref NP_626 780.1	glucarate dehydratase [Streptomyces coelicolor A3(2)]	20.19	1	1
2	212222 82 ref NP_628 061.1	DNA gyrase subunit B [Streptomyces coelicolor A3(2)]	14.79	1	59
3	212230 83 ref NP_628 862.1	50S ribosomal protein L4 [Streptomyces coelicolor A3(2)]	12.83	1	42
4	212205 46 ref NP_626 325.1	hypothetical protein SCO2065 [Streptomyces coelicolor A3(2)]	11.24	1	40
5	212239 15 ref NP_629 694.1	NAD(P)H-dependent glycerol-3-phosphate dehydrogenase [Streptomyces coelicolor A3(2)]	9.99	1	21
6	212220 26 ref NP_627 805.1	peptide hydrolase [Streptomyces coelicolor A3(2)]	7.50	1	12
7	212199 65 ref NP_625 744.1	transcriptional regulator [Streptomyces coelicolor A3(2)]	7.01	1	29
8	212200 62 ref NP_625 841.1	acetyltransferase [Streptomyces coelicolor A3(2)]	5.14	1	34
9	321412 70 ref NP_733	translation initiation factor IF-2 [Streptomyces coelicolor A3(2)]	4.45	1	48

	671.1				
10	212218 02 refl NP_627 581.1	Clp-family ATP-binding protease [Streptomyces coelicolor A3(2)]	4.41	2	31 35
11	212230 97 refl NP_628 876.1	50S ribosomal protein L6 [Streptomyces coelicolor A3(2)]	4.22	1	25
12	212220 44 refl NP_627 823.1	adenylosuccinate synthetase [Streptomyces coelicolor A3(2)]	3.70	1	23
13	P08779	Tax_Id=9606 Gene_Symbol=KRT16 Keratin, type I cytoskeletal 16	3.45	2	27 47
14	212239 80 refl NP_629 759.1	elongation factor Ts [Streptomyces coelicolor A3(2)]	3.42	1	49
15	212198 13 refl NP_625 592.1	hypothetical protein SCO1306 [Streptomyces coelicolor A3(2)]	3.36	1	13
16	212189 74 refl NP_624 753.1	peptidase [Streptomyces coelicolor A3(2)]	3.27	1	46
17	212258 36 refl NP_631 615.1	oxidoreductase [Streptomyces coelicolor A3(2)]	3.16	1	45
18	212210 92 refl NP_626 871.1	aminopeptidase [Streptomyces coelicolor A3(2)]	3.03	1	58
19	212235 79 refl NP_629 358.1	hypothetical protein SCO5211 [Streptomyces coelicolor A3(2)]	2.90	1	56
20	212238 34 refl NP_629 613.1	oligopeptide-binding lipoprotein [Streptomyces coelicolor A3(2)]	2.85	1	9
21	212203 40 refl NP_626 119.1	cob(I)yrinic acid a,c-diamide adenosyltransferase [Streptomyces coelicolor A3(2)]	2.62	1	3
22	212197 38 refl NP_625 517.1	reductase [Streptomyces coelicolor A3(2)]	2.61	1	38

23	212249 24 ref NP_630 703.1	protein kinase [Streptomyces coelicolor A3(2)]	2.50	2	20 33
24	Q99456	Tax_Id=9606 Gene_Symbol=KRT12 Keratin, type I cytoskeletal 12	2.26	1	41
25	212214 52 ref NP_627 231.1	hypothetical protein SCO3009 [Streptomyces coelicolor A3(2)]	2.12	1	24
26	212241 49 ref NP_629 928.1	transcriptional regulator NrdR [Streptomyces coelicolor A3(2)]	2.10	1	44
27	212199 92 ref NP_625 771.1	elongation factor P [Streptomyces coelicolor A3(2)]	2.04	1	36
28	212250 93 ref NP_630 872.1	2-amino-3-ketobutyrate coenzyme A ligase [Streptomyces coelicolor A3(2)]	1.88	1	57
29	212230 40 ref NP_628 819.1	30S ribosomal protein S12 [Streptomyces coelicolor A3(2)]	1.56	1	50
30	212231 06 ref NP_628 885.1	30S ribosomal protein S13 [Streptomyces coelicolor A3(2)]	1.56	1	5
31	212197 24 ref NP_625 503.1	6-phosphofructokinase [Streptomyces coelicolor A3(2)]	1.52	1	6
32	212210 94 ref NP_626 873.1	serine protease [Streptomyces coelicolor A3(2)]	1.22	1	43
33	212225 50 ref NP_628 329.1	5~-nucleotidase [Streptomyces coelicolor A3(2)]	1.19	1	17
34	212197 43 ref NP_625 522.1	urease subunit alpha [Streptomyces coelicolor A3(2)]	1.10	1	15
35	212210 46 ref NP_626 825.1	gamma-glutamyl kinase [Streptomyces coelicolor A3(2)]	1.03	1	7
36	212231	30S ribosomal protein S11 [Streptomyces	0.93	1	37

	07 ref NP_628 886.1	coelicolor A3(2)]			
37	212220 78 ref NP_627 857.1	regulatory protein [Streptomyces coelicolor A3(2)]	0.92	1	30
38	212230 85 ref NP_628 864.1	50S ribosomal protein L2 [Streptomyces coelicolor A3(2)]	0.91	1	18
39	212241 80 ref NP_629 959.1	DNA topoisomerase IV subunit A [Streptomyces coelicolor A3(2)]	0.79	1	54
40	212207 85 ref NP_626 564.1	methyltransferase [Streptomyces coelicolor A3(2)]	0.76	1	11
41	212231 41 ref NP_628 920.1	chaperonin GroEL [Streptomyces coelicolor A3(2)]	0.63	1	26
42	212204 43 ref NP_626 222.1	excinuclease ABC subunit A [Streptomyces coelicolor A3(2)]	0.62	1	10
43	212223 11 ref NP_628 090.1	hypothetical protein SCO3904 [Streptomyces coelicolor A3(2)]	0.61	1	8
44	212222 26 ref NP_628 005.1	branched-chain alpha-keto acid dehydrogenase E1 subunit beta [Streptomyces coelicolor A3(2)]	0.52	1	53
45	212240 06 ref NP_629 785.1	hypothetical protein SCO5655 [Streptomyces coelicolor A3(2)]	0.49	1	22
46	212244 94 ref NP_630 273.1	regulatory protein [Streptomyces coelicolor A3(2)]	0.44	1	32
47	212238 99 ref NP_629 678.1	hypothetical protein SCO5544 [Streptomyces coelicolor A3(2)]	0.37	1	16
48	321412 35 ref NP_733 636.1	formyltetrahydrofolate deformylase [Streptomyces coelicolor A3(2)]	0.20	1	2

49	212204 31 refl NP_626 210.1	phosphoglycerate kinase [Streptomyces coelicolor A3(2)]	0.16	1	51
50	212215 00 refl NP_627 279.1	dipeptidase [Streptomyces coelicolor A3(2)]	0.15	1	4
51	212231 08 refl NP_628 887.1	DNA-directed RNA polymerase subunit alpha [Streptomyces coelicolor A3(2)]	0.10	1	14
52	212247 73 refl NP_630 552.1	acyl-CoA dehydrogenase [Streptomyces coelicolor A3(2)]	0.08	1	52
53	212207 69 refl NP_626 548.1	hypothetical protein SCO2300 [Streptomyces coelicolor A3(2)]	0.05	1	55
54	P48668 P02538	Tax_Id=9606 Gene_Symbol=KRT6C Keratin, type II cytoskeletal 6C Tax_Id=9606 Gene_Symbol=KRT6A Keratin, type II cytoskeletal 6A	0.03 0.03	1 1	28 28
55	212205 38 refl NP_626 317.1	hypothetical protein SCO2057 [Streptomyces coelicolor A3(2)]	0.03	1	19
56	212241 64 refl NP_629 943.1	RNA polymerase sigma factor [Streptomyces coelicolor A3(2)]	0.02	1	39

Group Nr. By the rule of parsimony, we have gathered all proteins sharing the same identified peptides into a single group.

Accession Nr. The accession number from the searched database (DB).

Protein Name The protein name in the DB.

Protein Score Sum of the contributing peptide scores.

NOTE: This score can only be used to support the identification of **one** protein per group.

Unique PSMs. The number of unique peptide-spectrum matches that contribute to the protein assignment.

PSM Serial Nrs. Sequential number of assigned peptide (in the following table.)

Other Grp. If the protein is assigned to another group, that (those) group number(s).

Score (Other) Protein score (as above) for this protein in other group(s).

Assigned Peptides										
#	Sequence	PTM Site	Nr. Scans	Mascot Score	Expectation	Isolated Mass	Delta Mass	Charge State	Matched Ions	Scan Nr.
1	R.LAFDGGK.V	0.0000002.0	1	20.190	0.038	475.73	0.0	2	'4/12	10160
2	K.DTKPEEAR.V	0.002000000.0	1	0.200	2.4	630.30	5.2	2	'2/16	5906
3	-MPQGKPSVVPDDGLTTRQR.R	0.0000200000000000000.0	1	2.620	2.9	775.72	6.9	3	'3/36	14255
4	R.LSANGGMAMVTFVPK.F	0.000000101000002.0	1	0.150	3.5	599.96	4.0	3	'3/28	19041
5	R.AIAGKK.K	0.000022.0	1	1.560	4.6	537.28	1.2	2	'2/10	8272
6	R.GTDIEMVSLADAVESLKTPDAR.Y	0.000000000000000002000000.0	1	1.520	3.6	1330.66	0.1	2	'2/44	31996
7	R.AVARGLVNFDAKEMPRL	0.00000000000020000.0	1	1.030	5.2	1009.02	2.2	2	'2/30	12036
8	K.KGIQDPDVK.R	0.000000002.0	1	0.610	3	621.82	0.2	2	'2/16	9859
9	K.ACNPNGFKTTIAVR.N	0.000000002000000.0	1	2.850	2.5	960.47	3.4	2	'4/28	15449
10	R.KGEFVDLFADLQTKGYSR.A	0.2000000000000000000.0	1	0.620	3.5	773.05	4.5	3	'2/34	1093
11	R.AYHKLLVWDIMKKPLATR.V	0.000200000012200000.0	2	0.760	3.5	732.88	1.6	4	'3/34	29630
12	R.IKQVR.L	0.02000.0	1	7.500	1.3	443.76	0.9	2	'2/8	7598
13	K.RPEKSR.W	0.000200.0	1	3.360	2	508.27	1.3	2	'4/10	5244
14	R.TDFDKLIVDVETKQAMRPR.D	0.0000200000000000000.0	1	0.100	4.3	1261.14	0.5	2	'2/36	6526
15	K.GSTMSKESMRDQLR.A	0.00010200100000.0	1	1.100	0.78	950.93	2.1	2	'2/26	2062
16	M.QGRFK.R	0.00002.0	1	0.370	3.6	439.73	1.1	2	'2/8	7829
17	R.VTEVQPDGTTK.T	0.00000000002.0	1	1.190	2.6	709.34	2.5	2	'4/20	15247
18	R.HPVSPWGKKEGR.T	0.000000022000.0	1	0.910	3.9	932.46	1.7	2	'2/22	984
19	R.AMMRELLKTPEDEP.R.R	0.001000020000000.0	1	0.030	2.5	692.33	6.8	3	'2/28	12856
20	K.QKDVADALGLSHGR.I	0.020000000000000.0	1	1.470	2.6	570.62	6.2	3	'3/26	14288
21	R.MSEVIGDVAKVGA	0.000000000200000	7	9.990	0.45	601.9	3.0	3	'4/28	21340

	ER.I	.0				7				
22	K.KLFENGLYCR.A	0.2000000000.0	1	0.490	2.4	514.9 2	5.5	3	'2/18	3557
23	R.GIGPTYADKINR.V	0.000000002000.0	1	3.700	2.1	774.3 9	5.5	2	'3/22	13398
24	R.NLVQKGDAPPSKR. S	0.0000200000020.0	1	2.120	3.1	632.6 6	3.5	3	'4/24	15688
25	K.AKGVKYEGEVIR.R	0.020020000000.0	4	4.220	2.4	917.9 7	2.6	2	'2/22	2010
26	R.EKLQER.L	0.020000.0	2	0.630	8.2	523.2 7	5.3	2	'2/10	1018
27	K.EELAYLRKNHEEE MLALR.G	0.00000002000000 000.0	1	0.530	4.3	829.7 5	2.4	3	'3/34	25233
28	R.GEMALKDAKNK.L	0.00100200200.0	1	0.030	2.4	569.6 0	3.0	3	'4/20	10991
29	R.CITVKADQLR.R	0.0000200000.0	1	7.010	1.1	482.9 2	5.9	3	'3/18	9368
30	R.DKTLTERGVR.I	0.0200000000.0	1	0.920	5.6	473.2 5	2.8	3	'3/18	10718
31	K.KVLKEIR.T	0.0002000.0	1	1.290	1.9	564.8 4	0.7	2	'2/12	3087
32	R.ALDDTDALGLK.L	0.00000000002.0	1	0.440	6.1	458.2 5	6.3	3	'2/20	16301
33	R.FPELKPMRDAWR. K	0.000020100000.0	1	1.030	3.2	602.3 0	2.1	3	'3/22	22186
34	R.VTEDGAASIGK.L	0.00000000002.0	1	5.140	1.1	645.8 1	1.5	2	'3/20	10810
35	R.FLPDKAIDLIDEAG SRMR.I	0.00002000000000 000.0	1	3.120	2.8	764.0 6	6.9	3	'2/34	1613
36	K.IKVDTRTSYDYLGR. V	0.02000000000000.0	1	2.040	2.7	883.9 5	5.9	2	'2/24	1342
37	K.GSRKSTPFAAQMA AESALAR.R	0.00020000001000 0000.0	1	0.930	2.6	1098. 53	3.0	2	'2/36	1021
38	R.WPKDVRVVRA	0.002000000.0	1	2.610	2.1	699.3 9	5.7	2	'2/16	1343
39	R.QIESKTMSKLR.H	0.00002000200.0	1	0.020	6.9	903.9 5	4.8	2	'2/20	2046
40	R.VKDVVGRR.G	0.02000000.0	4	11.24 0	0.39	586.3 3	1.3	2	'2/14	2378
41	R.KDAEAWFIEK.S	0.0000000002.0	1	2.260	2.6	740.3 6	0.9	2	'2/18	8900
42	K.KMKAAALR.H	0.21200000.0	1	12.83 0	0.24	464.2 4	2.4	3	'4/14	13496
43	R.GVTIGILDSGVDLG HPALQKT	0.00000000000000 00002.0	1	1.220	3.1	1117. 10	4.7	2	'3/38	22060
44	R.SGVTEPFSRTKVIN GVR.K	0.000000000020000 00.0	1	2.100	3.5	697.3 7	1.7	3	'3/32	1842

45	R.AGLTALLGPDKVL WK.V	0.0000000000000002 .0	2	3.160	1.2	609.0 1	4.1	3	'4/28	20119
46	R.KVVHSVSAR.N	0.200000000.0	1	3.270	1.2	613.3 4	2.9	2	'5/16	13407
47	R.LAADDFRKYEHE LALR.Q	0.000000002000000 00.0	1	2.920	3.1	764.3 9	6.1	3	'3/32	2475
48	K.RNTKAR.L	0.000200.0	2	4.450	2.4	494.7 7	3.3	2	'3/10	338
49	M.ANYTAADVKKLR. E	0.000000002200.0	2	3.420	2	918.4 7	4.4	2	'2/22	2478
50	R.GGRVKDLPGVR.Y	0.0000200000.0	1	1.560	2.2	698.8 9	0.9	2	'2/20	943
51	- .MKTIDELLSEGVAGK R.V	0.1000000000000002 0.0	1	0.160	5.5	502.2 6	2.2	4	'2/30	12578
52	R.GAFSMSEPALGSD VSAISSKAVR.D	0.0000100000000000 00002000.0	1	0.080	2.8	842.7 4	3.4	3	'2/44	1521
53	- .MAAEKMALAKAINE SLR.R	0.000021000200000 00.0	1	0.520	5.2	783.7 2	3.5	3	'2/32	2070
54	R.ALPDARDGLKPVH R.R	0.00000000020000. 0	1	0.790	4.8	894.4 8	0.9	2	'2/26	967
55	R.EVVAGSVPDLLTL YGKLR.E	0.0000000000000000 0200.0	1	0.050	3.8	572.8 1	4.6	4	'2/36	17568
56	K.KDTLAR.I	0.200000.0	1	2.900	3.8	473.7 5	1.9	2	'3/10	17681
57	K.AKRLR.Y	0.02000.0	1	1.880	4.6	443.7 7	3.4	2	'3/8	15381
58	R.FKDAWITFANRR.K	0.020000000000.0	1	3.030	2.4	884.4 5	0.1	2	'2/22	1195
59	R.NAKDVR.F	0.002000.0	1	14.79 0	0.19	473.2 4	1.6	2	'3/10	13350
			76							

Serial (sequential) number for peptide.

Sequence Assigned peptide sequence. Periods (".") delimit the sequence for internal peptides.

PTM Site Location of the post-translational modification (PTM) in the peptide.
Modification codes: [1] Oxidation (M); [2] pupylation (K)

Nr. Scans The number of MS/MS scans that were matched to this peptide.

Mascot Score Score given to this peptide/spectrum match by Mascot.

Expectation The number of matches with equal or better scores that are expected to occur by chance alone.

Isolated Mass "Mass" in the Orbitrap analyzer.

Delta Mass Difference between the observed and theoretical masses, in ppm.

Charge State Inferred ionic state of the peptide.

Matched Ions Number of matched MS/MS ions, as reported by Mascot. NOTE:
Temporarily disabled.

Scan Nr. MS/MS scan number in the original Xcalibur RAW file.

Late Exponential

MS data file: Δprc Late Exponential (1).raw
Instrument type: ESI-FTICR
Search engine: Mascot
Parameter file: NCBI-Scoelicolor-FT-alkyl-oxid-tight-HCD.par
Search database: Scoelicolor_A32_20130406.fasta (16740 entries)
Enzyme specificity: Trypsin (2 missed cleavages allowed)
MS mass tolerance: 7 ppm; MS/MS tolerance 20 mmu
Fixed modifications: Carbamidomethyl (C)
Var. modifications: [1] Oxidation (M); [2] pupylation (K)
Number of spectra: 31335
Input PSMs: 31 'Target'; 1 'Decoy'; 3.2% FDR
Output PSMs: 31 (33 spectra were assigned to these unique PSMs.)
Output Proteins: 30 in 30 Protein Groups

Gr p N r.	Accession Number	Protein Name	Protein Score	Unique PSMs	PSM Serial Nrs.
1	21222670 ref NP_62 8449.1	tellurium resistance protein [Streptomyces coelicolor A3(2)]	8.05	1	27
2	21220021 ref NP_62 5800.1	hypothetical protein SCO1521 [Streptomyces coelicolor A3(2)]	8.04	1	22
3	21220303 ref NP_62 6082.1	GntR family transcriptional regulator [Streptomyces coelicolor A3(2)]	6.60	1	30
4	21224335 ref NP_63 0114.1	aconitase hydratase [Streptomyces coelicolor A3(2)]	6.21	1	15
5	21220260 ref NP_62 6039.1	pseudouridine synthase [Streptomyces coelicolor A3(2)]	4.08	1	3
6	21220655 ref NP_62 6434.1	dihydrolipoamide succinyltransferase [Streptomyces coelicolor A3(2)]	3.33	1	21
7	21219210	ferredoxin/ferredoxin-NADP reductase	3.27	1	29

	ref NP_62 4989.1	[Streptomyces coelicolor A3(2)]			
8	21224182 ref NP_62 9961.1	protease [Streptomyces coelicolor A3(2)]	2.91	1	31
9	21220041 ref NP_62 5820.1	regulator [Streptomyces coelicolor A3(2)]	2.91	1	24
10	21224431 ref NP_63 0210.1	nitrite/sulfite reductase [Streptomyces coelicolor A3(2)]	2.37	2	5 25
11	21223088 ref NP_62 8867.1	30S ribosomal protein S3 [Streptomyces coelicolor A3(2)]	1.95	1	9
12	21223085 ref NP_62 8864.1	50S ribosomal protein L2 [Streptomyces coelicolor A3(2)]	1.72	1	10
13	21220272 ref NP_62 6051.1	DNA repair protein [Streptomyces coelicolor A3(2)]	1.63	1	23
14	21219908 ref NP_62 5687.1	hypothetical protein SCO1404 [Streptomyces coelicolor A3(2)]	1.41	1	11
15	21223317 ref NP_62 9096.1	DNA-binding protein [Streptomyces coelicolor A3(2)]	1.19	1	7
16	21223817 ref NP_62 9596.1	enoyl-CoA hydratase [Streptomyces coelicolor A3(2)]	0.85	1	16
17	21222311 ref NP_62 8090.1	hypothetical protein SCO3904 [Streptomyces coelicolor A3(2)]	0.71	1	4
18	21221989 ref NP_62 7768.1	transcriptional regulator [Streptomyces coelicolor A3(2)]	0.63	1	6
19	21222153 ref NP_62 7932.1	response regulator [Streptomyces coelicolor A3(2)]	0.62	1	28
20	32141243 ref NP_73 3644.1	DNA-directed RNA polymerase subunit beta~ [Streptomyces coelicolor A3(2)]	0.55	1	26
21	21224924 ref NP_63 0703.1	protein kinase [Streptomyces coelicolor A3(2)]	0.54	1	20
22	21221240 ref NP_62 7019.1	glucosamine-fructose-6-phosphate aminotransferase [Streptomyces coelicolor A3(2)]	0.40	1	18
23	21220496 ref NP_62 6275.1	pyruvate kinase [Streptomyces coelicolor A3(2)]	0.35	1	17

24	21222718 ref NP_62 8497.1	hypothetical protein SCO4326 [Streptomyces coelicolor A3(2)]	0.34	1	8
25	21219724 ref NP_62 5503.1	6-phosphofructokinase [Streptomyces coelicolor A3(2)]	0.32	1	2
26	21222296 ref NP_62 8075.1	thioredoxin [Streptomyces coelicolor A3(2)]	0.30	1	12
27	32141143 ref NP_73 3534.1	ATP phosphoribosyltransferase [Streptomyces coelicolor A3(2)]	0.20	1	13
28	21224494 ref NP_63 0273.1	regulatory protein [Streptomyces coelicolor A3(2)]	0.15	1	19
29	21221535 ref NP_62 7314.1	phosphopyruvate hydratase [Streptomyces coelicolor A3(2)]	0.10	1	1
30	21223110 ref NP_62 8889.1	tRNA pseudouridine synthase A [Streptomyces coelicolor A3(2)]	0.07	1	14

Group Nr. By the rule of parsimony, we have gathered all proteins sharing the same identified peptides into a single group.

Accession Nr. The accession number from the searched database (DB).

Protein Name The protein name in the DB.

Protein Score Sum of the contributing peptide scores.

NOTE: This score can only be used to support the identification of **one** protein per group.

Unique PSMs. The number of unique peptide-spectrum matches that contribute to the protein assignment.

PSM Serial Nrs. Sequential number of assigned peptide (in the following table.)

Other Grp. If the protein is assigned to another group, that (those) group number(s).

Score (Other) Protein score (as above) for this protein in other group(s).

Assigned Peptides										
#	Sequence	PTM Site	Nr. Sca ns	Masc ot Score	Expect ation	Isolat ed Mass	Delt a Mass	Charg e Stat e	Match ed Ions	Scan Nr.
1	K.GVEKAVLAVIEQIG PELVGYDATEQR.L	0.000200000000000 000000000000.0	1	0.100	4.9	1009. 86	0.7	3	'2/50	1488
2	R.GTDIEMVSLADAV ESLKTVPDAR.Y	0.000000000000000 02000000.0	1	0.320	4.7	887.4 4	0.1	3	'3/44	31134

3	R.TAFGPITLGDQKSG WLRR.L	0.000000000002000 000.0	2	4.080	2.1	749.3 9	5.4	3	'3/34	1138
4	K.KGIQDPDVK.R	0.000000002.0	1	0.710	2.9	621.8 2	0.2	2	'3/16	8473
5	R.QKDGRYYVGFAPR. V	0.0200000000000.0	1	1.550	3.5	900.4 5	5.8	2	'2/24	2563
6	R.ETVNKALADFAQR GWLR.L	0.000020000000000 00.0	1	0.630	6.1	555.2 9	0.9	4	'3/32	23581
7	R.ARLKPEDVGLESYG R.Q	0.000200000000000 .0	1	1.190	4.4	967.0 0	5.6	2	'3/28	7729
8	R.LWAADTVPGGVGE IVVMPFHEIMPAVRD GK.V	0.000000000000000 00000000000002.0	1	0.340	3.4	859.4 4	4.3	4	'3/58	22789
9	K.AGAKGIKIQCGR.G.L	0.0002002000000.0	1	1.950	3.4	901.4 5	2.6	2	'3/24	22906
10	R.HPVSPWGKKEGR. T	0.000000022000.0	1	1.720	3	932.4 6	3.5	2	'2/22	738
11	R.FKWVASAL.R.A	0.020000000.0	1	1.410	4.3	660.8 6	5.2	2	'2/16	6827
12	K.LNIDENPGTAAK.Y	0.000000000002.0	1	0.300	3.4	743.3 6	2.4	2	'3/22	15476
13	R.AMVPAKEAQR.I	0.0100020000.0	1	0.200	4.3	680.3 4	3.1	2	'2/18	8439
14	R.LDLSYDGSEFSGW AKQAGGR.R.T	0.00000000000002 000000.0	1	0.070	3	1272. 11	5.5	2	'2/40	16598
15	K.AVEKGLTR.K	0.00020000.0	1	6.210	1.4	558.8 0	1.7	2	'3/14	5244
16	K.VFAAGADIKEMQV MDHAAMIAR.S	0.0000000200000 0001000.0	1	0.850	1.7	1317. 62	5.5	2	'2/42	26757
17	K.KDEDDL.R.W	0.2000000.0	1	0.350	0.92	567.2 6	1.6	2	'3/12	8944
18	R.DLEAKVPAR.F	0.000020000.0	1	0.400	4	621.3 3	3.5	2	'2/16	7363
19	R.ALDTDALGLK.L	0.0000000002.0	1	0.150	6.6	458.2 5	6.0	3	'2/20	15015
20	R.FPELKPMRDAWR. K	0.000020100000.0	2	0.540	3.8	602.3 0	1.6	3	'3/22	23520
21	R.WLKSVGDSVEEDE PLLEVSTD.K.V	0.002000000000000 0000000.0	1	3.330	2.1	1359. 66	5.0	2	'3/42	27891
22	K.KAVIDAKR.G	0.00000020.0	1	8.040	1.5	572.3 3	3.3	2	'4/14	6942
23	RVMLAVEVVFAGTD PVPTYLFDEVAGVG GK.A	0.010000000000000 0000000002.0	1	1.630	3	1677. 82	3.9	2	'3/58	19640
24	R.KALALMNTTVSCE LHLR.L	0.200001000000000 00.0	1	2.910	3.1	1108. 56	1.6	2	'2/32	14643
25	-MAATPPKPAATPR.	0.000002000000. 0	1	0.820	5.2	811.9 2	0.5	2	'3/26	13434

	R									
26	K.KIVVTPDDGSDETA FPISKR.A	0.2000000000000000 00020.0	1	0.550	3.4	1331. 16	4.7	2	'2/38	1232
27	- .MAVSLSKGGNVSLT K.E	0.1000002000000000 .0	1	8.050	0.78	875.9 6	1.9	2	'4/28	3522
28	R.LRGKVEDDPARPR. L	0.0002000000000.0	1	0.620	3.8	876.4 6	1.1	2	'2/24	1956
29	K.QADMVAKTLENW AIR.D	0.000100200000000 .0	1	3.270	2.2	1002. 99	4.0	2	'2/28	12781
30	R.LAAERRTEK.D	0.000000002.0	1	6.600	1.5	658.8 5	5.0	2	'3/16	10615
31	R.EEKGYTYGVRAFG QVLRS	0.002000000000000 00.0	1	2.910	3.1	1108. 56	1.5	2	'2/32	14643
			33							

Serial (sequential) number for peptide.

Sequence Assigned peptide sequence. Periods (".") delimit the sequence for internal peptides.

PTM Site Location of the post-translational modification (PTM) in the peptide.
Modification codes: [1] Oxidation (M); [2] pupylation (K)

Nr. Scans The number of MS/MS scans that were matched to this peptide.

Mascot Score Score given to this peptide/spectrum match by Mascot.

Expectation The number of matches with equal or better scores that are expected to occur by chance alone.

Isolated Mass "Mass" in the Orbitrap analyzer.

Delta Mass Difference between the observed and theoretical masses, in ppm.

Charge State Inferred ionic state of the peptide.

Matched Ions Number of matched MS/MS ions, as reported by Mascot. NOTE:
Temporarily disabled.

Scan Nr. MS/MS scan number in the original Xcalibur RAW file.

MS data file: Δprc Late Exponential (2).raw

Instrument type: ESI-FTICR

Search engine: Mascot

Parameter file: NCBI-Scoelicolor-FT-alkyl-oxid-tight-HCD.par

Search database: Scoelicolor_A32_20130406.fasta (16740 entries)

Enzyme specificity: Trypsin (2 missed cleavages allowed)

MS mass tolerance: 7 ppm; MS/MS tolerance 20 mmu

Fixed modifications: Carbamidomethyl (C)

Var. modifications: [1] Oxidation (M); [2] pupylation (K)

Number of spectra: 23322

Input PSMs: 18 'Target'; 1 'Decoy'; 5.6% FDR

Output PSMs: 18 (19 spectra were assigned to these unique PSMs.)

Output Proteins: 18 in 18 Protein Groups

<i>Gr p Nr.</i>	<i>Accession Number</i>	<i>Protein Name</i>	<i>Protein Score</i>	<i>Unique PSMs</i>	<i>PSM Serial Nrs.</i>
1	21220992 ref NP_62677 1.1	PhoH-like protein [Streptomyces coelicolor A3(2)]	24.03	1	9
2	32141176 ref NP_733578.1	hypothetical protein SCO2616 [Streptomyces coelicolor A3(2)]	10.74	1	10
3	21221831 ref NP_627610.1	cell division protein FtsH-like protein [Streptomyces coelicolor A3(2)]	6.36	1	7
4	21223579 ref NP_629358.1	hypothetical protein SCO5211 [Streptomyces coelicolor A3(2)]	6.01	1	18
5	P02768-1	Tax_Id=9606 Gene_Symbol=ALB Isoform 1 of Serum albumin precursor	4.84	1	14
6	32141243 ref NP_733644.1	DNA-directed RNA polymerase subunit beta~ [Streptomyces coelicolor A3(2)]	2.41	1	3
7	21225124 ref NP_630903.1	methylmalonyl-CoA mutase [Streptomyces coelicolor A3(2)]	2.29	1	11
8	21224904 ref NP_630683.1	hypothetical protein SCO6606 [Streptomyces coelicolor A3(2)]	2.15	1	12
9	21223027 ref NP_628806.1	aspartate aminotransferase [Streptomyces coelicolor A3(2)]	1.75	1	5
10	21221411 ref NP_627190.1	SsrA-binding protein [Streptomyces coelicolor A3(2)]	1.75	1	6
11	21223694 ref NP_629473.1	hypothetical protein SCO5333 [Streptomyces coelicolor A3(2)]	1.56	1	8
12	21218748 ref NP_624527.1	oxidoreductase [Streptomyces coelicolor A3(2)]	1.48	1	16
13	21220394 ref NP_626173.1	hypothetical protein SCO1907 [Streptomyces coelicolor A3(2)]	0.87	1	15
14	21221036 ref NP_626815.1	hypothetical protein SCO2577 [Streptomyces coelicolor A3(2)]	0.81	1	13
15	21223186 ref NP_628965.1	succinyl-CoA synthetase subunit beta [Streptomyces coelicolor A3(2)]	0.56	1	17

16	21223834 r ef NP_6296 13.1	oligopeptide-binding lipoprotein [Streptomyces coelicolor A3(2)]	0.33	1	1
17	21220355 r ef NP_6261 34.1	hydroxylase [Streptomyces coelicolor A3(2)]	0.18	1	2
18	21220021 r ef NP_6258 00.1	hypothetical protein SC01521 [Streptomyces coelicolor A3(2)]	0.10	1	4

Group Nr. By the rule of parsimony, we have gathered all proteins sharing the same identified peptides into a single group.

Accession Nr. The accession number from the searched database (DB).

Protein Name The protein name in the DB.

Protein Score Sum of the contributing peptide scores.

NOTE: This score can only be used to support the identification of **one** protein per group.

Unique PSMs. The number of unique peptide-spectrum matches that contribute to the protein assignment.

PSM Serial Nrs. Sequential number of assigned peptide (in the following table.)

Other Grp. If the protein is assigned to another group, that (those) group number(s).

Score (Other) Protein score (as above) for this protein in other group(s).

Assigned Peptides											
#	Sequence	PTM Site	Nr. Scans	Mascot Score	Expectation	Isolated Mass	Delta Mass	Charge State	Matched Ions	Scan Nr.	
1	K.ACNPNGFKTTIA VR.N	0.000000002000000 .0	1	0.330	4.4	960.47	3.4	2	'4/28	11716	
2	K.EIRSVFEVHKISEVF AK.L	0.000000000000000 02.0	1	0.180	4.9	1131.10	0.1	2	'2/32	16395	
3	R.SLATGK.L	0.000002.0	1	2.410	3.6	410.21	6.7	2	'4/10	5927	
4	K.LIKNIEVAAR.M	0.002000000.0	1	0.100	2.6	457.26	0.5	3	'3/18	24142	
5	R.IQKLLAEAR.D	0.002000000.0	1	1.750	3.3	642.87	4.4	2	'2/16	7098	
6	K.LIAQNKKAR.H	0.000000200.0	1	1.750	3.3	642.87	4.3	2	'2/16	7098	
7	K.EFLQEPAK.F	0.00000002.0	1	6.360	1.4	402.20	0.8	3	'3/14	4363	
8	R.VTSMVQRIVRSSAI ADTVK.A	0.000000000000000 0002.0	1	1.560	3	576.81	0.0	4	'3/36	13214	

9	K.AVQALQSK.Q	0.00000002.0	2	24.03 0	0.024	544.2 9	3.2	2	'4/14	7665
10	K.ISDPEAVLDK.F	0.0000000002.0	1	10.74 0	0.33	443.8 9	6.2	3	'3/18	4759
11	R.DQQAVDSALAALR K.A	0.00000000000002. 0	1	2.290	3.7	864.9 4	5.3	2	'3/26	13719
12	R.REDAAAVYNK.A	0.00000000002.0	1	2.150	1.8	690.3 3	2.7	2	'3/18	6447
13	R.LNKELGAKPVR.R	0.00200002000.0	1	0.810	3.6	570.9 7	6.2	3	'3/20	11062
14	K.ATKEQLKA	0.0020000.0	1	4.840	2.4	530.7 8	0.7	2	'4/12	6222
15	K.KVAKER.K	0.0002000.0	1	0.870	6.3	522.7 9	0.5	2	'2/12	5674
16	R.GFQVFNTSYPQVK R.R	0.00000000000020. 0	1	1.480	3.4	638.6 5	3.0	3	'3/26	12775
17	K.SVVKAQVKVGGR.G	0.000200000000.0	1	0.560	4.4	735.9 2	5.9	2	'2/22	10413
18	K.KDTLAR.I	0.200000.0	1	6.010	1.9	473.7 5	1.2	2	'3/10	11011
			19							

Serial (sequential) number for peptide.

Sequence Assigned peptide sequence. Periods (".") delimit the sequence for internal peptides.

PTM Site Location of the post-translational modification (PTM) in the peptide.
Modification codes: [1] Oxidation (M); [2] pupylation (K)

Nr. Scans The number of MS/MS scans that were matched to this peptide.

Mascot Score Score given to this peptide/spectrum match by Mascot.

Expectation The number of matches with equal or better scores that are expected to occur by chance alone.

Isolated Mass "Mass" in the Orbitrap analyzer.

Delta Mass Difference between the observed and theoretical masses, in ppm.

Charge State Inferred ionic state of the peptide.

Matched Ions Number of matched MS/MS ions, as reported by Mascot. NOTE:
Temporarily disabled.

Scan Nr. MS/MS scan number in the original Xcalibur RAW file.

MS data file: WT Late Exponential (1).raw

Instrument type: ESI-FTICR

Search engine: Mascot

Parameter file: NCBI-Scoelicolor-FT-alkyl-oxid-tight-HCD.par

Search database: Scoelicolor_A32_20130406.fasta (16740 entries)

Enzyme specificity: Trypsin (2 missed cleavages allowed)

MS mass tolerance: 7 ppm; MS/MS tolerance 20 mmu

Fixed modifications: Carbamidomethyl (C)

Var. modifications: [1] Oxidation (M); [2] pupylation (K)

Number of spectra: 35551

Input PSMs: 28 'Target'; 0 'Decoy'; 0.0% FDR

Output PSMs: 28 (49 spectra were assigned to these unique PSMs.)

Output Proteins: 28 in 28 Protein Groups

Gr p N. r.	Accession Number	Protein Name	Protein Score	Unique PSMs	PSM Serial Nrs.
1	21220992 ref NP_62 6771.1	PhoH-like protein [Streptomyces coelicolor A3(2)]	21.70	1	19
2	21220260 ref NP_62 6039.1	pseudouridine synthase [Streptomyces coelicolor A3(2)]	11.13	1	3
3	21223547 ref NP_62 9326.1	molybdopterin biosynthesis-like protein MoeZ [Streptomyces coelicolor A3(2)]	10.36	1	7
4	21223871 ref NP_62 9650.1	D-3-phosphoglycerate dehydrogenase [Streptomyces coelicolor A3(2)]	6.83	1	27
5	21223757 ref NP_62 9536.1	large Ala/Glu-rich protein [Streptomyces coelicolor A3(2)]	5.67	1	10
6	21224048 ref NP_62 9827.1	prolyl-tRNA synthetase [Streptomyces coelicolor A3(2)]	4.92	1	8
7	32141270 ref NP_73 3671.1	translation initiation factor IF-2 [Streptomyces coelicolor A3(2)]	4.70	1	26
8	21225061 ref NP_63 0840.1	1-deoxy-D-xylulose-5-phosphate synthase [Streptomyces coelicolor A3(2)]	4.58	1	21
9	21224760 ref NP_63 0539.1	ABC transporter ATP-binding protein [Streptomyces coelicolor A3(2)]	4.25	1	13
10	21223324 ref NP_62 9103.1	aldoketoreductase [Streptomyces coelicolor A3(2)]	4.06	1	2
11	21222469 ref NP_62 8248.1	DNA polymerase III subunits gamma and tau [Streptomyces coelicolor A3(2)]	2.99	1	24
12	21224164 ref NP_62 9943.1	RNA polymerase sigma factor [Streptomyces coelicolor A3(2)]	2.91	1	15
13	21220157	glycerol-3-phosphate dehydrogenase	2.61	1	17

	ref NP_62 5936.1	[Streptomyces coelicolor A3(2)]			
14	21219537 ref NP_62 5316.1	hypothetical protein SCO1020 [Streptomyces coelicolor A3(2)]	2.45	1	22
15	21220614 ref NP_62 6393.1	hypothetical protein SCO2137 [Streptomyces coelicolor A3(2)]	2.20	1	12
16	21221989 ref NP_62 7768.1	transcriptional regulator [Streptomyces coelicolor A3(2)]	2.17	1	4
17	21219602 ref NP_62 5381.1	aldolase [Streptomyces coelicolor A3(2)]	2.06	1	5
18	21221451 ref NP_62 7230.1	two-component system response regulator [Streptomyces coelicolor A3(2)]	1.85	1	14
19	21224581 ref NP_63 0360.1	sugar kinase [Streptomyces coelicolor A3(2)]	1.83	1	9
20	21224924 ref NP_63 0703.1	protein kinase [Streptomyces coelicolor A3(2)]	1.57	1	18
21	21219750 ref NP_62 5529.1	hypothetical protein SCO1241 [Streptomyces coelicolor A3(2)]	1.48	1	28
22	21221457 ref NP_62 7236.1	translation initiation factor [Streptomyces coelicolor A3(2)]	1.47	1	1
23	21221227 ref NP_62 7006.1	acetyl/propionyl CoA carboxylase subunit beta [Streptomyces coelicolor A3(2)]	1.27	1	16
24	21225836 ref NP_63 1615.1	oxidoreductase [Streptomyces coelicolor A3(2)]	1.26	1	25
25	21221240 ref NP_62 7019.1	glucosamine-fructose-6-phosphate aminotransferase [Streptomyces coelicolor A3(2)]	1.18	1	23
26	21223306 ref NP_62 9085.1	histidine ammonia-lyase [Streptomyces coelicolor A3(2)]	1.09	1	11
27	21221448 ref NP_62 7227.1	preprotein translocase subunit SecA [Streptomyces coelicolor A3(2)]	1.08	1	6
28	21224904 ref NP_63 0683.1	hypothetical protein SCO6606 [Streptomyces coelicolor A3(2)]	0.90	1	20

Group Nr. By the rule of parsimony, we have gathered all proteins sharing the same identified peptides into a single group.

Accession Nr. The accession number from the searched database (DB).

Protein Name The protein name in the DB.

Protein Score Sum of the contributing peptide scores.

NOTE: This score can only be used to support the identification of **one** protein per group.

Unique PSMs. The number of unique peptide-spectrum matches that contribute to the protein assignment.

PSM Serial Nrs. Sequential number of assigned peptide (in the following table.)

Other Grp. If the protein is assigned to another group, that (those) group number(s).

Score (Other) Protein score (as above) for this protein in other group(s).

Assigned Peptides											
#	Sequence	PTM Site	Nr. Sca ns	Masc ot Score	Expect ation	Isolat ed Mass	Delt a Mass	Ch a rge Stat e	Match ed Ions	Scan Nr.	
1	R.NGEDKRPTGIPALR.W	0.00002000000000.0	1	1.470	3.2	883.96	5.5	2	'2/26	10010	
2	R.GESEEMVKGKAIAGR.R	0.00000000200000.0	2	4.060	0.86	559.60	0.2	3	'3/26	22239	
3	R.TAFGPITLGDQKSGWLRR.L	0.0000000000020000.0	5	11.130	0.42	749.39	5.4	3	'4/34	3963	
4	R.ETVNKALADFAQR.GWLR.L	0.0000200000000000.0	2	2.170	4.4	555.29	4.2	4	'3/32	38703	
5	-MNPPKTDAR.R	0.100020000.0	1	2.060	1.3	430.20	1.9	3	'3/16	5995	
6	K.LMRAGEGKILR.K	0.00000002000.0	3	1.080	5.4	496.27	6.5	3	'2/20	35048	
7	K.TGVRSAEVLAVLKS	0.0000000000002.0	3	10.360	0.29	529.30	3.3	3	'3/24	25826	
8	K.GLVWSKEVAPADVHVVAAGK.A	0.0000000000000000.00002.0	1	4.920	1.5	1138.60	1.5	2	'2/38	37182	
9	K.RGKYGVAGEFGHMQVVPGGHR.C	0.0020000000000100.000000.0	1	1.830	3.2	625.31	3.0	4	'3/40	13434	
10	R.IVAEAAEKAR.T	0.0000000200.0	1	5.670	2.1	650.84	2.3	2	'4/18	3067	
11	R.KLRTAVDNLAR.V	0.200000000000.0	1	1.090	3.9	750.42	2.6	2	'2/20	10996	
12	R.QRIGEKFR.D	0.00000200.0	1	2.200	4.3	638.84	2.3	2	'2/14	8861	
13	R.HVDDAEGKVAR.G	0.00000002000.0	1	4.250	1.1	720.35	2.8	2	'4/20	5559	

14	R.MPKRGGIEACTSIK.E	0.1000000000000002.0	1	1.850	4.5	903.95	4.5	2	'3/26	13139
15	R.RAKNHLLEANLR.L	0.002000000000.0	2	2.910	1.4	559.98	1.1	3	'2/22	37025
16	R.GKLLPRDR.V	0.02000000.0	1	1.270	3	599.34	4.7	2	'2/14	19551
17	R.TAPWKA	0.00002.0	1	2.610	1.3	423.21	5.8	2	'2/8	5103
18	R.FPELKPMRDAWR.K	0.000020100000.0	6	1.570	2.8	602.30	2.0	3	'3/22	25421
19	K.AVQALQSK.Q	0.0000002.0	1	21.700	0.042	544.29	1.0	2	'4/14	9452
20	R.REDAAAVYNK.A	0.000000002.0	1	0.900	3	690.33	1.2	2	'2/18	8030
21	K.LLTGRQDFSKLRS	0.00000000200.0	1	4.580	1.5	559.64	0.3	3	'2/22	13350
22	M.SKGSNTPVPTTALRVELGWR.S	0.0200000000000000.00000.0	1	2.450	3.1	603.82	2.0	4	'3/38	18194
23	K.KLAAQYAEAR.S	0.2000000000.0	1	1.180	3.5	682.35	2.7	2	'2/18	6723
24	R.EKAFFGPASSRYK.I	0.0200000000000.0	1	2.990	2.1	865.93	1.8	2	'2/24	8142
25	R.AGLTALLGPDKVLWK.V	0.000000000000002.0	2	1.260	2.2	609.01	2.4	3	'4/28	20330
26	K.RNTKAR.L	0.000200.0	4	4.700	2.2	494.77	4.3	2	'3/10	19258
27	K.LKVVAR.A	0.020000.0	1	6.830	0.88	464.78	0.2	2	'3/10	10491
28	R.GMVIIRWLTAECGGKLR.V	0.010000000000002.00.0	2	1.480	4.1	555.54	1.9	4	'3/32	20867
			49							

Serial (sequential) number for peptide.

Sequence Assigned peptide sequence. Periods (".") delimit the sequence for internal peptides.

PTM Site Location of the post-translational modification (PTM) in the peptide.
Modification codes: [1] Oxidation (M); [2] pupylation (K)

Nr. Scans The number of MS/MS scans that were matched to this peptide.

Mascot Score Score given to this peptide/spectrum match by Mascot.

Expectation The number of matches with equal or better scores that are expected to occur by chance alone.

Isolated Mass "Mass" in the Orbitrap analyzer.

Delta Mass Difference between the observed and theoretical masses, in ppm.

Charge State Inferred ionic state of the peptide.

Matched Ions Number of matched MS/MS ions, as reported by Mascot. NOTE: Temporarily disabled.

Scan Nr. MS/MS scan number in the original Xcalibur RAW file.

MS data file: WT Late Exponential (2).raw
Instrument type: ESI-FTICR
Search engine: Mascot
Parameter file: NCBI-Scoelicolor-FT-alkyl-oxid-tight-HCD.par
Search database: Scoelicolor_A32_20130406.fasta (16740 entries)
Enzyme specificity: Trypsin (2 missed cleavages allowed)
MS mass tolerance: 7 ppm; MS/MS tolerance 20 mmu
Fixed modifications: Carbamidomethyl (C)
Var. modifications: [1] Oxidation (M); [2] pupylation (K)
Number of spectra: 22198
Input PSMs: 2 'Target'; 0 'Decoy'; 0.0% FDR
Output PSMs: 2 (2 spectra were assigned to these unique PSMs.)
Output Proteins: 2 in 2 Protein Groups

<i>Gr p N r.</i>	<i>Accession Number</i>	<i>Protein Name</i>	<i>Protein Score</i>	<i>Unique PSMs</i>	<i>PSM Serial Nrs.</i>
1	21220251 r ef NP_6260 30.1	GTP-binding protein EngA [Streptomyces coelicolor A3(2)]	2.39	1	2
2	21222670 r ef NP_6284 49.1	tellurium resistance protein [Streptomyces coelicolor A3(2)]	0.12	1	1

Group Nr. By the rule of parsimony, we have gathered all proteins sharing the same identified peptides into a single group.

Accession Nr. The accession number from the searched database (DB).

Protein Name The protein name in the DB.

Protein Score Sum of the contributing peptide scores.

NOTE: This score can only be used to support the identification of **one** protein per group.

Unique PSMs. The number of unique peptide-spectrum matches that contribute to the protein assignment.

PSM Serial Nrs. Sequential number of assigned peptide (in the following table.)

Other Grp. If the protein is assigned to another group, that (those) group number(s).

Score (Other) Protein score (as above) for this protein in other group(s).

Assigned Peptides

#	Sequence	PTM Site	Nr. Scans	Mascot Score	Expectation	Isolated Mass	Delta Mass	Charge State	Matched Ions	Scan Nr.
1	- .MAVSLSKGGNVSLT K.E	0.1000002000000000 .0	1	0.120	5	584.30	3.2	3	'2/28	15783
2	R.ILFGTQAGTKPPR.F	0.0000000002000.0	1	2.390	2.9	543.63	3.9	3	'2/24	22048
			2							

Serial (sequential) number for peptide.
Sequence Assigned peptide sequence. Periods (".") delimit the sequence for internal peptides.
PTM Site Location of the post-translational modification (PTM) in the peptide.
 Modification codes: [1] Oxidation (M); [2] pupylation (K)
Nr. Scans The number of MS/MS scans that were matched to this peptide.
Mascot Score Score given to this peptide/spectrum match by Mascot.
Expectation The number of matches with equal or better scores that are expected to occur by chance alone.
Isolated Mass "Mass" in the Orbitrap analyzer.
Delta Mass Difference between the observed and theoretical masses, in ppm.
Charge State Inferred ionic state of the peptide.
Matched Ions Number of matched MS/MS ions, as reported by Mascot. NOTE:
 Temporarily disabled.
Scan Nr. MS/MS scan number in the original Xcalibur RAW file.

Stationary

MS data file: Δprc Stationary (1).raw
 Instrument type: ESI-FTICR
 Search engine: Mascot
 Parameter file: NCBI-Scoelicolor-FT-alkyl-oxid-tight-HCD.par
 Search database: Scoelicolor_A32_20130406.fasta (16740 entries)
 Enzyme specificity: Trypsin (2 missed cleavages allowed)
 MS mass tolerance: 7 ppm; MS/MS tolerance 20 mmu
 Fixed modifications: Carbamidomethyl (C)
 Var. modifications: [1] Oxidation (M); [2] pupylation (K)
 Number of spectra: 27656
 Input PSMs: 24 'Target'; 0 'Decoy'; 0.0% FDR
 Output PSMs: 24 (49 spectra were assigned to these unique PSMs.)
 Output Proteins: 24 in 23 Protein Groups

<i>Group N. Nr.</i>	<i>Accession Number</i>	<i>Protein Name</i>	<i>Protein Score</i>	<i>Unique PSMs</i>	<i>PSM Serial Nrs.</i>
1	21220992 ref NP_62 6771.1	PhoH-like protein [Streptomyces coelicolor A3(2)]	22.06	1	11
2	21221001 ref NP_62 6780.1	glucarate dehydratase [Streptomyces coelicolor A3(2)]	18.98	1	2
3	21221513 ref NP_62 7292.1	allantoate amidohydrolase [Streptomyces coelicolor A3(2)]	9.41	1	23
4	21224053 ref NP_62 9832.1	transcription elongation factor NusA [Streptomyces coelicolor A3(2)]	7.17	1	7
5	21218770 ref NP_62 4549.1	nitrate reductase subunit alpha NarG2 [Streptomyces coelicolor A3(2)]	3.72	2	17 21
6	21221779 ref NP_62 7558.1	hypothetical protein SCO3349 [Streptomyces coelicolor A3(2)]	3.21	1	15
7	21221372 ref NP_62 7151.1	oxidoreductase subunit [Streptomyces coelicolor A3(2)]	2.67	1	8
8	21223281 ref NP_62 9060.1	transcriptional regulator [Streptomyces coelicolor A3(2)]	2.25	1	9
9	32141335 ref NP_73 3736.1	oxidoreductase, partial [Streptomyces coelicolor A3(2)]	1.96	1	6
10	P20930	Tax_Id=9606 Gene_Symbol=FLG Filaggrin	1.96	1	14
11	21223533 ref NP_62 9312.1	hypothetical protein SCO5164 [Streptomyces coelicolor A3(2)]	1.83	1	22
12	P19013	Tax_Id=9606 Gene_Symbol=KRT4 keratin 4	1.48	1	16
13	21221989 ref NP_62 7768.1	transcriptional regulator [Streptomyces coelicolor A3(2)]	1.16	1	5
14	P50446	Tax_Id=10090 Gene_Symbol=Krt6a Keratin, type II cytoskeletal 6A	0.81	1	19
15	32141142 ref NP_73 3533.1	hypothetical protein SCO1407, partial [Streptomyces coelicolor A3(2)]	0.72	1	1
16	P05784	Tax_Id=10090 Gene_Symbol=Krt18 Keratin, type I cytoskeletal 18	0.59	1	12
17	21223631 ref NP_62	hypothetical protein SCO5264 [Streptomyces coelicolor A3(2)]	0.58	1	4

	9410.1				
18	21224042 ref NP_62 9821.1	acyl CoA dehydrogenase [Streptomyces coelicolor A3(2)]	0.53	1	20
19	Q9QWL7	Tax_Id=10090 Gene_Symbol=Krt17 Keratin, type I cytoskeletal 17	0.52	1	18
	Q04695	Tax_Id=9606 Gene_Symbol=KRT17 Keratin, type I cytoskeletal 17	0.52	1	18
20	21224182 ref NP_62 9961.1	protease [Streptomyces coelicolor A3(2)]	0.49	1	24
21	21220313 ref NP_62 6092.1	subtilisin-like protease [Streptomyces coelicolor A3(2)]	0.39	1	10
22	21224618 ref NP_63 0397.1	hydrolase [Streptomyces coelicolor A3(2)]	0.08	1	3
23	21225124 ref NP_63 0903.1	methylmalonyll-CoA mutase [Streptomyces coelicolor A3(2)]	0.06	1	13

Group Nr. By the rule of parsimony, we have gathered all proteins sharing the same identified peptides into a single group.

Accession Nr. The accession number from the searched database (DB).

Protein Name The protein name in the DB.

Protein Score Sum of the contributing peptide scores.

NOTE: This score can only be used to support the identification of **one** protein per group.

Unique PSMs. The number of unique peptide-spectrum matches that contribute to the protein assignment.

PSM Serial Nrs. Sequential number of assigned peptide (in the following table.)

Other Grp. If the protein is assigned to another group, that (those) group number(s).

Score (Other) Protein score (as above) for this protein in other group(s).

Assigned Peptides										
#	Sequence	PTM Site	Nr. Scans	Mascot Score	Expectation	Isolated Mass	Delta Mass	Charge State	Matched Ions	Scan Nr.
1	R.LGKDRELAAR.L	0.0020000000.0	1	0.720	6.7	457.92	3.4	3	'2/18	19964
2	R.LAFDGGK.V	0.0000002.0	1	18.980	0.046	475.73	0.6	2	'4/12	9071
3	R.TKYGDDR.V	0.0200000.0	1	0.080	1.2	549.2	1.9	2	'2/12	5059

						5				
4	K.QEWKEQAR.R	0.00020000.0	1	0.580	3.1	659.3 1	3.1	2	'3/14	3555
5	R.ETVNKALADFAQR GWLR.L	0.000020000000000 00.0	3	1.160	5.1	555.2 9	5.8	4	'2/32	22401
6	-.MKKPPRDEPR.D	0.1220000000.0	1	1.960	1.8	878.4 2	6.6	2	'2/18	4053
7	R.VAKGVR.G	0.002000.0	1	7.170	2	436.7 5	0.6	2	'3/10	6130
8	K.KEWLAR.E	0.200000.0	3	2.670	4.2	523.2 8	1.1	2	'2/10	1619
9	R.LRAKVEDVPSSPTL IR.T	0.000200000000000 0.0	1	2.250	2.3	1012. 55	5.4	2	'3/30	14974
10	K.NGVGMTGVAPGVK VAGIK.V	0.000010000000200 000.0	1	0.390	5.4	479.2 6	2.9	4	'2/34	21233
11	K.AVQALQSK.Q	0.00000002.0	2	22.06 0	0.04	544.2 9	0.4	2	'4/14	8271
12	R.DWGHYFKIIEDLR. A	0.0000002000000.0	1	0.590	4.8	645.6 6	6.4	3	'2/24	29323
13	R.DQQAVDSALAALR K.A	0.00000000000002. 0	1	0.060	6.4	576.9 6	6.8	3	'3/26	16985
14	R.KRPSSLERR.N	0.200000000.0	3	1.960	5.1	457.9 2	4.2	3	'3/16	22948
15	K.KAKDEK.S	0.002000.0	1	3.210	3.2	481.2 5	6.2	2	'2/10	3333
16	K.NTKSEIAELNRMIQ R.L	0.00200000001000 .0	1	1.480	4.3	1031. 52	1.9	2	'2/28	27135
17	K.YMLDLSRGGPTIW MSLQDAEK.I	0.010000000000010 000002.0	1	3.620	1.4	896.0 9	2.5	3	'2/40	7948
18	R.TKFETEQALR.M	0.0200000000.0	1	0.520	3.7	489.2 5	5.0	3	'2/18	14487
19	R.GKLEGLEDALQK.A	0.000000000002.0	1	0.810	6.3	515.2 7	5.7	3	'2/22	18362
20	R.LSLPAMCVGAGKW CLKIAR.E	0.000001000002000 0000.0	1	0.530	5.7	598.3 1	1.7	4	'3/36	25264
21	R.TVNVPKTEVGGKR. G	0.0000020000020.0	1	0.100	6.3	468.4 9	3.9	4	'2/24	15117
22	R.LGNLNANNQQK.G	0.00000000002.0	1	1.830	2.4	728.8 6	3.6	2	'3/20	9137
23	R.REAQLAGAVATFG K.I	0.0000000000002. 0	19	9.410	0.61	831.4 4	2.7	2	'3/26	22148
24	R.EEKGYTYGVRAFG QVLRS	0.002000000000000 00.0	1	0.490	5.4	1108. 56	1.5	2	'2/32	14166
			49							

Serial (sequential) number for peptide.

Sequence Assigned peptide sequence. Periods (".") delimit the sequence for internal peptides.
PTM Site Location of the post-translational modification (PTM) in the peptide.
 Modification codes: [1] Oxidation (M); [2] pupylation (K)
Nr. Scans The number of MS/MS scans that were matched to this peptide.
Mascot Score Score given to this peptide/spectrum match by Mascot.
Expectation The number of matches with equal or better scores that are expected to occur by chance alone.
Isolated Mass "Mass" in the Orbitrap analyzer.
Delta Mass Difference between the observed and theoretical masses, in ppm.
Charge State Inferred ionic state of the peptide.
Matched Ions Number of matched MS/MS ions, as reported by Mascot. NOTE:
 Temporarily disabled.
Scan Nr. MS/MS scan number in the original Xcalibur RAW file.

MS data file: Δprc Stationary (2).raw
 Instrument type: ESI-FTICR
 Search engine: Mascot
 Parameter file: NCBI-Scoelicolor-FT-alkyl-oxid-tight-HCD.par
 Search database: Scoelicolor_A32_20130406.fasta (16740 entries)
 Enzyme specificity: Trypsin (2 missed cleavages allowed)
 MS mass tolerance: 7 ppm; MS/MS tolerance 20 mmu
 Fixed modifications: Carbamidomethyl (C)
 Var. modifications: [1] Oxidation (M); [2] pupylation (K)
 Number of spectra: 24778
 Input PSMs: 16 'Target'; 2 'Decoy'; 12.5% FDR
 Output PSMs: 16 (19 spectra were assigned to these unique PSMs.)
 Output Proteins: 16 in 16 Protein Groups

<i>Gr p N r.</i>	<i>Accession Number</i>	<i>Protein Name</i>	<i>Protein Score</i>	<i>Unique PSMs</i>	<i>PSM Serial Nrs.</i>
1	21220992 ref NP_62 6771.1	PhoH-like protein [Streptomyces coelicolor A3(2)]	20.98	1	11
2	21218783 ref NP_62 4562.1	TetR family transcriptional regulator [Streptomyces coelicolor A3(2)]	7.64	1	3
3	32141312 ref NP_73 3712.1	phospholipase C, partial [Streptomyces coelicolor A3(2)]	7.64	1	4
4	21221221 ref NP_62 7000.1	acetolactate synthase [Streptomyces coelicolor A3(2)]	5.34	1	7

5	21223104 ref NP_62 8883.1	translation initiation factor IF-1 [Streptomyces coelicolor A3(2)]	5.19	1	8
6	21224957 ref NP_63 0736.1	glucose-6-phosphate 1-dehydrogenase [Streptomyces coelicolor A3(2)]	3.92	1	13
7	21225093 ref NP_63 0872.1	2-amino-3-ketobutyrate coenzyme A ligase [Streptomyces coelicolor A3(2)]	2.16	1	16
8	21221243 ref NP_62 7022.1	AraC family transcription regulator [Streptomyces coelicolor A3(2)]	1.88	1	5
9	21225737 ref NP_63 1516.1	phenylacetate-CoA ligase [Streptomyces coelicolor A3(2)]	1.71	1	6
10	21225286 ref NP_63 1065.1	isocitrate dehydrogenase [Streptomyces coelicolor A3(2)]	1.61	1	15
11	21224494 ref NP_63 0273.1	regulatory protein [Streptomyces coelicolor A3(2)]	1.02	1	10
12	32141190 ref NP_73 3591.1	phosphoribosylaminoimidazole carboxylase ATPase subunit [Streptomyces coelicolor A3(2)]	0.71	1	1
13	21220031 ref NP_62 5810.1	threonyl-tRNA synthetase [Streptomyces coelicolor A3(2)]	0.39	1	14
14	P02533	Tax_Id=9606 Gene_Symbol=KRT14 Keratin, type I cytoskeletal 14	0.31	1	2
15	21222374 ref NP_62 8153.1	Xaa-Pro aminopeptidase [Streptomyces coelicolor A3(2)]	0.26	1	12
16	21220156 ref NP_62 5935.1	glycerol kinase [Streptomyces coelicolor A3(2)]	0.19	1	9

Group Nr. By the rule of parsimony, we have gathered all proteins sharing the same identified peptides into a single group.

Accession Nr. The accession number from the searched database (DB).

Protein Name The protein name in the DB.

Protein Score Sum of the contributing peptide scores.

NOTE: This score can only be used to support the identification of **one** protein per group.

Unique PSMs. The number of unique peptide-spectrum matches that contribute to the protein assignment.

PSM Serial Nrs. Sequential number of assigned peptide (in the following table.)

Other Grp. If the protein is assigned to another group, that (those) group

number(s).

Score (Other) Protein score (as above) for this protein in other group(s).

Assigned Peptides										
#	Sequence	PTM Site	Nr. Scans	Mascot Score	Expectation	Isolated Mass	Delta Mass	Charge State	Matched Ions	Scan Nr.
1	R.KRPVNR.W	0.200000.0	1	0.710	2	506.79	0.1	2	'2/10	7665
2	K.EELAYLKKNHEEE MNALR.G	0.000000220000000 000.0	2	0.310	3.1	1352.15	5.8	2	'2/34	14549
3	R.KGDVR.E	0.20000.0	2	7.640	1.3	409.21	2.3	2	'2/8	4300
4	R.TGTDAKR.G	0.0000020.0	1	7.640	0.67	496.25	3.7	2	'3/12	8625
5	- .MSHDSTAAPEAAAR KLSGR.R	0.000000000000002 0000.0	1	1.880	2.8	1100.03	1.3	2	'2/36	14492
6	R.KVTGRCDDMIILR. G	0.2000000000000.0	1	1.710	3.4	910.46	1.4	2	'2/24	9746
7	R.ADAAKK.L	0.000002.0	1	5.340	2	423.72	0.5	2	'3/10	6022
8	- .MAKKQGAIEIEGTVV ESLPNAMFK.V	0.002200000000000 000000100.0	1	5.190	1.3	774.14	4.9	4	'3/46	26414
9	R.TDALCKELGRNVG QDR.F	0.000002000000000	1	0.190	4.1	1038.00	0.4	2	'2/30	14053
10	R.ALLDTDALGLK.L	0.0000000002.0	1	1.020	5.3	458.25	6.5	3	'2/20	13671
11	K.AVQALQSK.Q	0.00000002.0	2	20.980	0.051	544.29	0.7	2	'4/14	7810
12	R.FPGERLVIPAGNLK. T	0.0000000000002.	1	0.260	3.7	877.49	4.1	2	'3/26	18804
13	R.KAVEELDASR.G	0.2000000000.0	1	3.920	2.1	680.84	1.8	2	'4/18	8750
14	K.KMQEIQK.R	0.0100002.0	1	0.390	4.8	582.29	5.6	2	'2/12	5810
15	R.STEKSAVIAEDGTL R.I	0.000200000000000 .0	1	1.610	3.5	910.46	5.2	2	'2/28	9746
16	K.AKRLR.Y	0.02000.0	1	2.160	4.5	443.76	0.5	2	'3/8	14612
			19							

Serial (sequential) number for peptide.

Sequence Assigned peptide sequence. Periods (".") delimit the sequence for internal peptides.
PTM Site Location of the post-translational modification (PTM) in the peptide.
 Modification codes: [1] Oxidation (M); [2] pupylation (K)
Nr. Scans The number of MS/MS scans that were matched to this peptide.
Mascot Score Score given to this peptide/spectrum match by Mascot.
Expectation The number of matches with equal or better scores that are expected to occur by chance alone.
Isolated Mass "Mass" in the Orbitrap analyzer.
Delta Mass Difference between the observed and theoretical masses, in ppm.
Charge State Inferred ionic state of the peptide.
Matched Ions Number of matched MS/MS ions, as reported by Mascot. NOTE:
 Temporarily disabled.
Scan Nr. MS/MS scan number in the original Xcalibur RAW file.

MS data file: WT Stationary (1).raw
 Instrument type: ESI-FTICR
 Search engine: Mascot
 Parameter file: NCBI-Scoelicolor-FT-alkyl-oxid-tight-HCD.par
 Search database: Scoelicolor_A32_20130406.fasta (16740 entries)
 Enzyme specificity: Trypsin (2 missed cleavages allowed)
 MS mass tolerance: 7 ppm; MS/MS tolerance 20 mmu
 Fixed modifications: Carbamidomethyl (C)
 Var. modifications: [1] Oxidation (M); [2] pupylation (K)
 Number of spectra: 27946
 Input PSMs: 33 'Target'; 0 'Decoy'; 0.0% FDR
 Output PSMs: 33 (55 spectra were assigned to these unique PSMs.)
 Output Proteins: 34 in 33 Protein Groups

<i>Gr p N r.</i>	<i>Accession Number</i>	<i>Protein Name</i>	<i>Protein Score</i>	<i>Unique PSMs</i>	<i>PSM Serial Nrs.</i>
1	21220992 ref NP_62 6771.1	PhoH-like protein [Streptomyces coelicolor A3(2)]	25.44	1	15
2	21221513 ref NP_62 7292.1	allantoate amidohydrolase [Streptomyces coelicolor A3(2)]	12.30	1	32
3	21222670 ref NP_62 8449.1	tellurium resistance protein [Streptomyces coelicolor A3(2)]	10.52	1	25
4	32141142 ref NP_73 3533.1	hypothetical protein SCO1407, partial [Streptomyces coelicolor A3(2)]	8.70	1	2
5	21223231	succinate dehydrogenase iron-sulfur	6.42	1	30

	ref NP_62 9010.1	subunit [Streptomyces coelicolor A3(2)]			
6	21222494 ref NP_62 8273.1	ATP-dependent helicase [Streptomyces coelicolor A3(2)]	5.70	1	12
7	21223096 ref NP_62 8875.1	30S ribosomal protein S8 [Streptomyces coelicolor A3(2)]	5.30	1	4
8	21221735 ref NP_62 7514.1	arginyl-tRNA synthetase [Streptomyces coelicolor A3(2)]	4.26	1	31
9	32141261 ref NP_73 3662.1	transcription termination factor Rho [Streptomyces coelicolor A3(2)]	4.23	1	11
10	21224474 ref NP_63 0253.1	hypothetical protein SCO6148 [Streptomyces coelicolor A3(2)]	3.29	1	9
11	21223325 ref NP_62 9104.1	TetR family transcriptional regulator [Streptomyces coelicolor A3(2)]	2.65	1	16
12	A2A5Y0	Tax_Id=10090 Gene_Symbol=Krt31 keratin complex 1, acidic, gene 1	2.56	1	8
13	32141194 ref NP_73 3595.1	penicillin acylase, partial [Streptomyces coelicolor A3(2)]	2.28	1	5
14	21222227 ref NP_62 8006.1	branched-chain alpha-keto acid dehydrogenase E1 subunit alpha, partial [Streptomyces coelicolor A3(2)]	1.92	1	6
15	21224182 ref NP_62 9961.1	protease [Streptomyces coelicolor A3(2)]	1.79	1	33
16	21220343 ref NP_62 6122.1	precorrin-4 C11-methyltransferase [Streptomyces coelicolor A3(2)]	1.45	1	26
17	21220485 ref NP_62 6264.1	DNA polymerase I [Streptomyces coelicolor A3(2)]	1.44	1	7
18	Q5D862	Tax_Id=9606 Gene_Symbol=FLG2 Filaggrin-2	1.26	1	29
19	21222946 ref NP_62 8725.1	NADH dehydrogenase subunit B [Streptomyces coelicolor A3(2)]	1.23	1	19
20	21225061 ref NP_63 0840.1	1-deoxy-D-xylulose-5-phosphate synthase [Streptomyces coelicolor A3(2)]	1.12	1	24
21	21221718 ref NP_62 7497.1	hypothetical protein SCO3286 [Streptomyces coelicolor A3(2)]	1.10	1	1
22	21224924	protein kinase [Streptomyces coelicolor]	1.04	1	14

	ref NP_63 0703.1	A3(2)]			
23	21218702 ref NP_62 4481.1	hypothetical protein SC00143 [Streptomyces coelicolor A3(2)]	0.86	1	27
24	21221230 ref NP_62 7009.1	acyl-CoA dehydrogenase [Streptomyces coelicolor A3(2)]	0.69	1	10
25	21223186 ref NP_62 8965.1	succinyl-CoA synthetase subunit beta [Streptomyces coelicolor A3(2)]	0.66	1	28
26	21221386 ref NP_62 7165.1	oxidoreductase [Streptomyces coelicolor A3(2)]	0.60	1	13
27	21220013 ref NP_62 5792.1	GTP pyrophosphokinase [Streptomyces coelicolor A3(2)]	0.25	1	17
28	21224713 ref NP_63 0492.1	DNA recombinase [Streptomyces coelicolor A3(2)]	0.24	1	20
29	P20930	Tax_Id=9606 Gene_Symbol=FLG Filaggrin	0.21	1	23
30	21220438 ref NP_62 6217.1	excinuclease ABC subunit C [Streptomyces coelicolor A3(2)]	0.21	1	3
31	21225448 ref NP_63 1227.1	GntR family transcriptional regulator [Streptomyces coelicolor A3(2)]	0.07	1	21
32	21223429 ref NP_62 9208.1	exodeoxyribonuclease VII large subunit [Streptomyces coelicolor A3(2)]	0.04	1	22
33	Q9UE12	Type I hair keratin 1 - Homo sapiens (Human).	0.03	1	18
	Q15323	Keratin, type I cuticular HA1 (Hair keratin, type I HA1)	0.03	1	18

Group Nr. By the rule of parsimony, we have gathered all proteins sharing the same identified peptides into a single group.

Accession Nr. The accession number from the searched database (DB).

Protein Name The protein name in the DB.

Protein Score Sum of the contributing peptide scores.

NOTE: This score can only be used to support the identification of **one** protein per group.

Unique PSMs. The number of unique peptide-spectrum matches that contribute to the protein assignment.

PSM Serial Nrs. Sequential number of assigned peptide (in the following table.)

Other Grp. If the protein is assigned to another group, that (those) group number(s).

Score (Other) Protein score (as above) for this protein in other group(s).

Assigned Peptides										
#	Sequence	PTM Site	Nr. Scans	Mascot Score	Expectation	Isolated Mass	Delta Mass	Charge State	Matched Ions	Scan Nr.
1	K.SADLEAQAKLR.M	0.00000000200.0	1	1.100	4.7	722.87	4.4	2	'2/20	9582
2	R.LGKDRELAAR.L	0.0020000000.0	4	8.700	0.96	457.92	2.4	3	'3/18	17874
3	R.FAITYQRAK.R	0.000000002.0	1	0.210	4.1	447.57	2.4	3	'2/16	14364
4	R.ISKPGLR.V	0.0020000.0	1	5.300	0.77	507.29	0.4	2	'3/12	11549
5	K.TGKKATVETAAPDR.G	0.00220000000000.0	2	2.280	2.4	644.32	3.1	3	'3/26	29472
6	R.AAWEAKDPLRL	0.00000200000.0	1	1.920	2.4	504.93	5.7	3	'2/20	13834
7	K.KTDSTSGGRPRLMLMDGHSLAYR.A	0.20000000000000010000000.0	1	1.440	2.7	1404.67	6.7	2	'2/44	7161
8	R.LASYMEKVR.Q	0.000000200.0	1	2.560	1.9	670.34	3.9	2	'2/16	9423
9	R.YAKAIEEHFPGR.W	0.002000000000.0	1	3.290	1.8	830.91	1.3	2	'3/22	14444
10	M.DHKLSPELEELR.R	0.002000000000.0	1	0.690	3.7	854.93	1.6	2	'2/22	1686
11	R.KLADKR.I	0.000020.0	1	4.230	2.7	487.27	1.6	2	'4/10	4891
12	R.KPEAR.A	0.20000.0	1	5.700	0.67	422.22	0.9	2	'4/8	4159
13	R.AAKMVR.T	0.002100.0	1	0.600	6.2	467.74	5.0	2	'2/10	6174
14	R.FPELKPMRDAWR.K	0.000020100000.0	6	1.040	3.1	602.30	1.8	3	'3/22	20573
15	K.AVQALQSK.Q	0.00000002.0	2	25.440	0.018	544.29	1.7	2	'4/14	9148
16	K.DGEAATGQAASRP.K.R	0.00000000000002.0	1	2.650	1.5	801.38	0.8	2	'2/26	9900
17	K.SSGKSDDHLNDMAWLR.Q	0.000202000000000.0	2	0.250	1.2	816.04	0.1	3	'2/32	2884
18	K.LAADDFRKYQTELSLR.Q	0.000000002000000.0	1	0.030	4.9	757.38	6.9	3	'2/32	1201
19	R.EAAAALKALPTIEMKG	0.00000002000001.0	1	1.230	4.3	1002.00	1.5	2	'2/30	14234
20	R.KTPRPFDMMVVVNE	0.200000010000000	1	0.240	5.3	668.6	3.7	3	'3/28	18684

	GR.G	.0				7				
21	R.AKVQDMR.E	0.0200010.0	1	0.070	3.7	553.7 7	0.2	2	'3/12	6256
22	R.VVVHAKPEWYAPR .G	0.0000020000000.0	1	0.040	5.4	897.9 6	5.4	2	'2/24	16645
23	R.KRPSSLERR.N	0.200000000.0	1	0.210	6.8	457.9 2	5.8	3	'2/16	17874
24	K.LLTGRQDFSKLR.S	0.000000000200.0	1	1.120	2.9	559.6 4	1.1	3	'2/22	13048
25	- .MAVSLSKGGNVSLT K.E	0.100000200000000 .0	3	10.52 0	0.44	584.3 1	1.8	3	'3/28	26241
26	R.EFAKHGTMAVFL SAARS	0.000200000000000 00.0	1	1.450	3.9	520.7 6	4.9	4	'3/32	19751
27	K.TFGSKRGLYLTALR .R	0.000020000000000.	1	0.860	5.2	913.4 9	7.0	2	'2/26	17520
28	K.VEKPLVVRLDGNN AELGR.K	0.002000000000000 000.0	1	0.660	3.4	1111. 60	1.8	2	'2/34	3082
29	R.INKSHISPSR.E	0.0020000000.0	1	1.260	3.7	691.3 6	4.0	2	'4/18	9477
30	K.AIAEVKRA	0.0000020.0	1	6.420	1.5	515.2 9	1.8	2	'3/12	10246
31	K.TKANPRE	0.020000.0	1	4.260	1.4	465.2 5	7.0	2	'3/10	6246
32	R.REAQLAGAVATFG K.I	0.0000000000002.	10	12.30 0	0.33	831.4 4	1.4	2	'3/26	21276
33	R.EEKGYTYGVRAFG QVLR.S	0.002000000000000 00.0	1	1.790	4	1108. 56	1.5	2	'2/32	15193
			55							

Serial (sequential) number for peptide.

Sequence Assigned peptide sequence. Periods (".") delimit the sequence for internal peptides.

PTM Site Location of the post-translational modification (PTM) in the peptide.
Modification codes: [1] Oxidation (M); [2] pupylation (K)

Nr. Scans The number of MS/MS scans that were matched to this peptide.

Mascot Score Score given to this peptide/spectrum match by Mascot.

Expectation The number of matches with equal or better scores that are expected to occur by chance alone.

Isolated Mass "Mass" in the Orbitrap analyzer.

Delta Mass Difference between the observed and theoretical masses, in ppm.

Charge State Inferred ionic state of the peptide.

Matched Ions Number of matched MS/MS ions, as reported by Mascot. NOTE:
Temporarily disabled.

Scan Nr. MS/MS scan number in the original Xcalibur RAW file.

MS data file: WT Stationary (2).raw
 Instrument type: ESI-FTICR
 Search engine: Mascot
 Parameter file: NCBI-Scoelicolor-FT-alkyl-oxid-tight-HCD.par
 Search database: Scoelicolor_A32_20130406.fasta (16740 entries)
 Enzyme specificity: Trypsin (2 missed cleavages allowed)
 MS mass tolerance: 7 ppm; MS/MS tolerance 20 mmu
 Fixed modifications: Carbamidomethyl (C)
 Var. modifications: [1] Oxidation (M); [2] pupylation (K)
 Number of spectra: 28315
 Input PSMs: 35 'Target'; 1 'Decoy'; 2.9% FDR
 Output PSMs: 35 (59 spectra were assigned to these unique PSMs.)
 Output Proteins: 34 in 33 Protein Groups

<i>Gr p N r.</i>	<i>Accession Number</i>	<i>Protein Name</i>	<i>Protein Score</i>	<i>Unique PSMs</i>	<i>PSM Serial Nrs.</i>
1	21221001 ref NP_62 6780.1	glucarate dehydratase [Streptomyces coelicolor A3(2)]	26.58	1	4
2	21220992 ref NP_62 6771.1	PhoH-like protein [Streptomyces coelicolor A3(2)]	16.85	1	18
3	21221513 ref NP_62 7292.1	allantoate amidohydrolase [Streptomyces coelicolor A3(2)]	8.85	1	35
4	21218783 ref NP_62 4562.1	TetR family transcriptional regulator [Streptomyces coelicolor A3(2)]	8.63	1	10
5	21219604 ref NP_62 5383.1	hypothetical protein SC01089 [Streptomyces coelicolor A3(2)]	7.31	1	29
6	21221779 ref NP_62 7558.1	hypothetical protein SC03349 [Streptomyces coelicolor A3(2)]	6.30	1	22
7	21223083 ref NP_62 8862.1	50S ribosomal protein L4 [Streptomyces coelicolor A3(2)]	5.85	1	25
8	21221989 ref NP_62 7768.1	transcriptional regulator [Streptomyces coelicolor A3(2)]	5.50	1	11
9	21219724 ref NP_62 5503.1	6-phosphofructokinase [Streptomyces coelicolor A3(2)]	5.48	2	8 16
10	21225286 ref NP_63	isocitrate dehydrogenase [Streptomyces coelicolor A3(2)]	4.28	1	31

	1065.1				
11	21222670 ref NP_62 8449.1	tellurium resistance protein [Streptomyces coelicolor A3(2)]	4.08	1	27
12	21220144 ref NP_62 5923.1	ATPase AAA [Streptomyces coelicolor A3(2)]	3.16	1	7
13	21225782 ref NP_63 1561.1	heat shock protein 90 [Streptomyces coelicolor A3(2)]	3.13	1	5
14	21219442 ref NP_62 5221.1	succinate dehydrogenase flavoprotein subunit [Streptomyces coelicolor A3(2)]	2.94	2	13 17
15	21219984 ref NP_62 5763.1	carbamoyl phosphate synthase large subunit [Streptomyces coelicolor A3(2)]	2.93	1	26
16	21223192 ref NP_62 8971.1	bifunctional phosphoribosylaminoimidazolecarboxamide formyltransferase/IMP cyclohydrolase [Streptomyces coelicolor A3(2)]	2.87	1	33
17	21220006 ref NP_62 5785.1	30S ribosomal protein S4 [Streptomyces coelicolor A3(2)]	2.02	1	21
18	21221072 ref NP_62 6851.1	folylypolyglutamate synthase [Streptomyces coelicolor A3(2)]	2.02	1	34
19	21220395 ref NP_62 6174.1	large hypothetical protein [Streptomyces coelicolor A3(2)]	1.88	1	24
20	P60712	(Bos taurus) Actin, cytoplasmic 1	1.86	1	1
21	21220485 ref NP_62 6264.1	DNA polymerase I [Streptomyces coelicolor A3(2)]	1.86	1	12
22	21223757 ref NP_62 9536.1	large Ala/Glu-rich protein [Streptomyces coelicolor A3(2)]	1.66	1	32
23	21223758 ref NP_62 9537.1	hypothetical protein SC05398 [Streptomyces coelicolor A3(2)]	1.66	1	23
24	21219544 ref NP_62 5323.1	lyase [Streptomyces coelicolor A3(2)]	0.91	1	28
25	21221073 ref NP_62 6852.1	valyl-tRNA synthetase [Streptomyces coelicolor A3(2)]	0.74	1	14
26	21222648 ref NP_62 8427.1	hypothetical protein SC04253 [Streptomyces coelicolor A3(2)]	0.61	1	3
27	21225448	GntR family transcriptional regulator	0.57	1	20

	ref NP_63 1227.1	[Streptomyces coelicolor A3(2)]			
28	21221189 ref NP_62 6968.1	type II citrate synthase [Streptomyces coelicolor A3(2)]	0.51	1	6
29	21224591 ref NP_63 0370.1	oxidoreductase alpha-subunit [Streptomyces coelicolor A3(2)]	0.25	1	9
	21222978 ref NP_62 8757.1	oxidoreductase [Streptomyces coelicolor A3(2)]	0.25	1	9
30	Q7Z794	Tax_Id=9606 Gene_Symbol=KRT77 Keratin 77	0.14	1	30
31	32141239 ref NP_73 3640.1	hypothetical protein SCO4494 [Streptomyces coelicolor A3(2)]	0.09	1	2
32	21223149 ref NP_62 8928.1	inosine 5~ monophosphate dehydrogenase [Streptomyces coelicolor A3(2)]	0.03	1	15
33	21224242 ref NP_63 0021.1	RNA methyltransferase [Streptomyces coelicolor A3(2)]	0.01	1	19

Group Nr. By the rule of parsimony, we have gathered all proteins sharing the same identified peptides into a single group.

Accession Nr. The accession number from the searched database (DB).

Protein Name The protein name in the DB.

Protein Score Sum of the contributing peptide scores.

NOTE: This score can only be used to support the identification of **one** protein per group.

Unique PSMs. The number of unique peptide-spectrum matches that contribute to the protein assignment.

PSM Serial Nrs. Sequential number of assigned peptide (in the following table.)

Other Grp. If the protein is assigned to another group, that (those) group number(s).

Score (Other) Protein score (as above) for this protein in other group(s).

Assigned Peptides										
#	Sequence	PTM Site	Nr. Scans	Mascot Score	Expectation	Isolated Mass	Delta Mass	Charge State	Matched Ions	Scan Nr.
1	R.DIKEKLCYVALDFE QEMATAASSSLEK.S	0.002020000000000 0100000000000.0	1	1.860	1.2	1222.57	3.3	3	'2/54	12655
2	K.DGKVR.N	0.00200.0	1	0.090	8.1	409.2	1.2	2	'2/8	5168

						1				
3	R.GVHKAPANEVVR.G	0.000200000000.0	1	0.610	4.9	507.2 7	1.4	3	'2/22	17906
4	R.LAFDGGK.V	0.0000002.0	1	26.58 0	0.0087	475.7 3	0.9	2	'4/12	9479
5	R.SVAKGEIDLSGTEA DKSDAEK.E	0.000000000000000 200000.0	1	3.130	1.6	798.3 8	2.5	3	'4/40	21480
6	K.EDGVRLMFGFHRV YK.N	0.000000100000002 .0	1	0.510	4.1	675.0 0	2.0	3	'3/28	1546
7	K.DFLDKNQKGRL.V	0.00002002000.0	1	3.160	2.1	910.4 5	0.3	2	'2/20	10571
8	R.GTDIEMVSLADAV ESLKTVPDAR.Y	0.000000000000000 02000000.0	1	2.030	3.1	887.4 4	1.1	3	'5/44	1061
9	R.YDKVVVPEMNLGQ LATLIR.A	0.002000000000000 0000.0	1	0.250	4.9	801.4 3	0.3	3	'2/36	3502
10	R.KGDVR.E	0.20000.0	2	8.630	1	409.2 1	5.4	2	'2/8	4413
11	R.ETVNKALADFAQR GWLR.L	0.000020000000000 00.0	2	5.500	2	555.2 9	0.9	4	'4/32	29742
12	K.KTDSTSGGRPRLM LMDGHSLAYR.A	0.200000000000001 00000000.0	1	1.860	2.4	1404. 67	6.7	2	'2/44	7283
13	R.KAVEAKYGNLFDM YQR.I	0.000002000000100 0.0	1	0.290	3.6	1096. 53	4.0	2	'2/30	3312
14	R.ELGKEGKSR.H	0.000200200.0	1	0.740	4.6	745.3 7	5.8	2	'2/16	12318
15	R.ISGPVPTDGAGKLL GIVTNRDMAFETDR. S	0.000000000002000 0000001000000.0	1	0.030	4.4	798.6 6	1.3	4	'2/54	27524
16	K.RFAIVVAAEGAKPK .A	0.00000000000002. 0	1	3.450	2.2	567.3 2	4.6	3	'3/26	17601
17	R.IWVPKAK.G	0.0000202.0	1	2.650	3.2	664.3 5	5.8	2	'2/12	11943
18	K.AVQALQSK.Q	0.00000002.0	2	16.85 0	0.13	544.2 9	2.1	2	'4/14	30420
19	R.LKGEVVAEQLQR.L	0.020000000000.0	1	0.010	6.1	538.2 9	0.1	3	'2/22	14419
20	R.AKVQDMR.E	0.0200010.0	1	0.570	3.3	553.7 7	0.4	2	'2/12	6034
21	K.TNMKTGEALVIEL ERR.L	0.000200000000000 0.0	1	2.020	2.6	701.7 0	2.8	3	'2/30	3777
22	K.KAKDEK.S	0.002000.0	7	6.300	1.6	481.2 5	6.8	2	'2/10	3922
23	R.DKGVR.V	0.02000.0	3	1.660	5.2	409.2 1	5.4	2	'2/8	4413
24	-MASKSSAR.L	0.00020000.0	1	1.880	1.5	540.7 6	3.5	2	'2/14	6375
25	K.KMKAAALR.H	0.21200000.0	1	5.850	1.2	464.2 4	4.0	3	'4/14	12319

26	K.KGSQFTFVGEPGD KDELLR.E	0.2000000000000000 0000.0	1	2.930	2.3	789.3 9	2.9	3	'2/36	4024
27	- .MAVSLSKGGNVSLT K.E	0.1000002000000000 .0	1	4.080	2.1	584.3 1	1.1	3	'5/28	25813
28	R.MMKVPDAASVAA VRSLER.A	0.0020000000000000 000.0	1	0.910	4.7	725.3 7	4.7	3	'2/34	3970
29	R.VVEHPAWPVLKDA VER.I	0.0000000000200000 0.0	1	7.310	0.91	696.7 0	5.4	3	'4/30	6075
30	R.LQAEISNVKK.Q	0.0000000002.0	1	0.140	5.5	686.8 8	0.1	2	'3/18	15356
31	R.STEKSAVIAEDGTL R.I	0.0002000000000000 .0	1	4.280	1.6	910.4 5	5.8	2	'2/28	10571
32	K.AAKTAEDVLNK.A	0.0020000002.0	1	1.660	2.9	823.4 0	4.7	2	'3/20	8906
33	R.RALVSVYDKTGLE DLAR.G	0.0000000020000000 00.0	1	2.870	2.5	717.0 4	6.1	3	'2/32	5200
34	K.QDATVILAQQPVD AAQVMLKK.A	0.0000000000000000 001002.0	1	2.020	2.8	632.3 4	5.9	4	'2/40	5525
35	R.REAQLAGAVATFG K.I	0.0000000000000002. 0	14	8.850	0.68	831.4 4	3.9	2	'3/26	22262
			59							

Serial (sequential) number for peptide.

Sequence Assigned peptide sequence. Periods (".") delimit the sequence for internal peptides.

PTM Site Location of the post-translational modification (PTM) in the peptide.
Modification codes: [1] Oxidation (M); [2] pupylation (K)

Nr. Scans The number of MS/MS scans that were matched to this peptide.

Mascot Score Score given to this peptide/spectrum match by Mascot.

Expectation The number of matches with equal or better scores that are expected to occur by chance alone.

Isolated Mass "Mass" in the Orbitrap analyzer.

Delta Mass Difference between the observed and theoretical masses, in ppm.

Charge State Inferred ionic state of the peptide.

Matched Ions Number of matched MS/MS ions, as reported by Mascot. NOTE:
Temporarily disabled.

Scan Nr. MS/MS scan number in the original Xcalibur RAW file.

MS data file: Unenriched WT 2.raw

Instrument type: ESI-FTICR

Search engine: Mascot

Parameter file: NCBI-Scoelicolor-FT-alkyl-oxid-tight-HCD.par

Search database: Scoelicolor_A32_20130406.fasta (16740 entries)

Enzyme specificity: Trypsin (2 missed cleavages allowed)
 MS mass tolerance: 7 ppm; MS/MS tolerance 20 mmu
 Fixed modifications: Carbamidomethyl (C)
 Var. modifications: [1] Oxidation (M); [2] pupylation (K)
 Number of spectra: 27318
 Input PSMs: 4 'Target'; 0 'Decoy'; 0.0% FDR
 Output PSMs: 4 (4 spectra were assigned to these unique PSMs.)
 Output Proteins: 4 in 4 Protein Groups

Protein IDs							
G rp N r.	Access ion Numbe r	Protein Name	Prot ein Sco re	Uniq ue PSM s	PSM Serial Nrs.	Ot her Gr p.	Sc ore (oth er)
1	2122318 7 ref NP _628966 .1	succinyl-CoA synthetase subunit alpha [Streptomyces coelicolor A3(2)]	8.12	1	4		
2	2122199 8 ref NP _627777 .1	hypothetical protein SCO3581 [Streptomyces coelicolor A3(2)]	5.00	1	2		
3	2122318 6 ref NP _628965 .1	succinyl-CoA synthetase subunit beta [Streptomyces coelicolor A3(2)]	4.66	1	3		
4	Q6NXH 9	Tax_Id=10090 Gene_Symbol=Krt73 Keratin 73	2.31	1	1		

Group Nr. By the rule of parsimony, we have gathered all proteins sharing the same identified peptides into a single group.

Accession Nr. The accession number from the searched database (DB).

Protein Name The protein name in the DB.

Protein Score Sum of the contributing peptide scores.

NOTE: This score can only be used to support the identification of **one** protein per group.

Unique PSMs. The number of unique peptide-spectrum matches that contribute to the protein assignment.

PSM Serial Nrs. Sequential number of assigned peptide (in the following table.)

Other Grp. If the protein is assigned to another group, that (those) group number(s).

Score (Other) Protein score (as above) for this protein in other group(s).

Assigned Peptides										
#	Sequence	PTM Site	Nr. Sc ans	Mas cot Scor e	Expect ation	Isola ted Mas s	Delt a Mas s	Cha rge Stat e	Matc hed Ions	Scan Nr.

1	K.KQCSNLETAIADAE QR.G	0.2000000000000000.	1	2.310	1.4	1038. 99	5.4	2	'3/30	10753
2	K.VIIREAK.K	0.0000002.0	1	5.000	2.4	536.3 2	6.8	2	'3/12	15432
3	K.VADILVK.L	0.0000002.0	1	4.660	2.6	500.7 9	3.6	2	'3/12	13123
4	K.KGNKTR.I	0.000200.0	1	8.120	0.68	473.7 6	3.0	2	'4/10	9834
			4							

Serial (sequential) number for peptide.
Sequence Assigned peptide sequence. Periods (".") delimit the sequence for internal peptides.
PTM Site Location of the post-translational modification (PTM) in the peptide.
Modification codes: [1] Oxidation (M); [2] pupylation (K)
Nr. Scans The number of MS/MS scans that were matched to this peptide.
Mascot Score Score given to this peptide/spectrum match by Mascot.
Expectation The number of matches with equal or better scores that are expected to occur by chance alone.
Isolated Mass "Mass" in the Orbitrap analyzer.
Delta Mass Difference between the observed and theoretical masses, in ppm.
Charge State Inferred ionic state of the peptide.
Matched Ions Number of matched MS/MS ions, as reported by Mascot. NOTE: Temporarily disabled.
Scan Nr. MS/MS scan number in the original Xcalibur RAW file.

MS data file: Unenriched WT 1.raw
 Instrument type: ESI-FTICR
 Search engine: Mascot
 Parameter file: NCBI-Scoelicolor-FT-alkyl-oxid-tight-HCD.par
 Search database: Scoelicolor_A32_20130406.fasta (16740 entries)
 Enzyme specificity: Trypsin (2 missed cleavages allowed)
 MS mass tolerance: 7 ppm; MS/MS tolerance 20 mmu
 Fixed modifications: Carbamidomethyl (C)
 Var. modifications: [1] Oxidation (M); [2] pupylation (K)
 Number of spectra: 30893
 Input PSMs: 32 'Target'; 4 'Decoy'; 12.5% FDR
 Output PSMs: 32 (36 spectra were assigned to these unique PSMs.)
 Output Proteins: 30 in 30 Protein Groups

Protein IDs									
Group Number	Accession Number	Protein Name		Protein Score	Unique PSMs	PSM Serial Nrs.		Other Group.	Score (other)
1	2122123 4 ref NP_627013	monooxygenase [Streptomyces coelicolor A3(2)]		13.4 1	1	17			

	.1						
2	2122110 0 ref NP _626879 .1	aminopeptidase N [Streptomyces coelicolor A3(2)]	12.6 3	1	28		
3	2122002 1 ref NP _625800 .1	hypothetical protein SCO1521 [Streptomyces coelicolor A3(2)]	10.9 5	1	22		
4	2122001 3 ref NP _625792 .1	GTP pyrophosphokinase [Streptomyces coelicolor A3(2)]	9.56	1	2		
5	2122196 2 ref NP _627741 .1	DNA topoisomerase I [Streptomyces coelicolor A3(2)]	7.45	2	12 19		
6	2122317 5 ref NP _628954 .1	ATP-dependent DNA helicase II [Streptomyces coelicolor A3(2)]	7.26	1	10		
7	2122369 3 ref NP _629472 .1	DNA methylase [Streptomyces coelicolor A3(2)]	5.48	1	23		
8	3214127 0 ref NP _733671 .1	translation initiation factor IF-2 [Streptomyces coelicolor A3(2)]	5.46	1	6		
9	2122323 1 ref NP _629010 .1	succinate dehydrogenase iron-sulfur subunit [Streptomyces coelicolor A3(2)]	4.26	1	29		
10	2122206 2 ref NP _627841 .1	hypothetical protein SCO3647 [Streptomyces coelicolor A3(2)]	4.03	1	13		
11	2122388 4 ref NP _629663 .1	alpha-isopropylmalate/homocitrate synthase family transferase [Streptomyces coelicolor A3(2)]	3.87	2	3 32		
12	2121998 4 ref NP _625763 .1	carbamoyl phosphate synthase large subunit [Streptomyces coelicolor A3(2)]	2.78	1	30		
13	2122314 1 ref NP _628920 .1	chaperonin GroEL [Streptomyces coelicolor A3(2)]	2.69	1	8		
14	2122356 8 ref NP _629347 .1	hypothetical protein SCO5199 [Streptomyces coelicolor A3(2)]	2.33	1	16		
15	2122223 1 ref NP _628010 .1	Ser/Thr protein kinase [Streptomyces coelicolor A3(2)]	2.09	1	5		

16	2122310 6 ref NP _628885 .1	30S ribosomal protein S13 [Streptomyces coelicolor A3(2)]	1.14	1	4			
17	2122318 6 ref NP _628965 .1	succinyl-CoA synthetase subunit beta [Streptomyces coelicolor A3(2)]	1.11	1	31			
18	2122044 2 ref NP _626221 .1	fructokinase [Streptomyces coelicolor A3(2)]	1.09	1	26			
19	2122375 7 ref NP _629536 .1	large Ala/Glu-rich protein [Streptomyces coelicolor A3(2)]	1.08	1	20			
20	2122599 2 ref NP _631771 .1	transcriptional regulator [Streptomyces coelicolor A3(2)]	1.06	1	27			
21	2122060 6 ref NP _626385 .1	hypothetical protein SCO2129 [Streptomyces coelicolor A3(2)]	1.04	1	15			
22	2122424 2 ref NP _630021 .1	RNA methyltransferase [Streptomyces coelicolor A3(2)]	0.73	1	25			
23	2122578 9 ref NP _631568 .1	chaperone [Streptomyces coelicolor A3(2)]	0.72	1	1			
24	2122391 5 ref NP _629694 .1	NAD(P)H-dependent glycerol-3-phosphate dehydrogenase [Streptomyces coelicolor A3(2)]	0.70	1	14			
25	2121992 4 ref NP _625703 .1	hypothetical protein SCO1421 [Streptomyces coelicolor A3(2)]	0.70	1	7			
26	2122198 2 ref NP _627761 .1	acetyl-CoA synthetase [Streptomyces coelicolor A3(2)]	0.67	1	9			
27	2122065 5 ref NP _626434 .1	dihydrolipoamide succinyltransferase [Streptomyces coelicolor A3(2)]	0.48	1	24			
28	2122321 3 ref NP _628992 .1	serine hydroxymethyltransferase [Streptomyces coelicolor A3(2)]	0.38	1	11			
29	2122230 0 ref NP _628079 .1	hypothetical protein SCO3893 [Streptomyces coelicolor A3(2)]	0.17	1	21			
30	2122504	nucleotide sugar-1-phosphate transferase	0.17	1	18			

6 ref NP_630825 .1	[Streptomyces coelicolor A3(2)]						
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Group Nr. By the rule of parsimony, we have gathered all proteins sharing the same identified peptides into a single group.

Accession Nr. The accession number from the searched database (DB).

Protein Name The protein name in the DB.

Protein Score Sum of the contributing peptide scores.

NOTE: This score can only be used to support the identification of **one** protein per group.

Unique PSMs. The number of unique peptide-spectrum matches that contribute to the protein assignment.

PSM Serial Nrs. Sequential number of assigned peptide (in the following table.)

Other Grp. If the protein is assigned to another group, that (those) group number(s).

Score (Other) Protein score (as above) for this protein in other group(s).

Assigned Peptides											
#	Sequence	PTM Site	Nr. Scans	Mscot Score	Expectation	Isolated Mass	Delta Mass	Charge State	Matched Ions	Scan Nr.	
1	R.VHAQGMTLKVT AK.K	0.000001002000000.0	1	0.720	5	461.49	1.4	4	'3/28	24528	
2	R.KMVVAMAKDPR.V	0.00000002000.0	1	9.560	0.63	744.88	6.5	2	'5/20	10161	
3	R.MLVSDMAGRASIE LKGK.E	0.1000010000000020 0.0	1	0.450	4.1	1041.02	1.8	2	'2/32	16095	
4	R.AIAGKK.K	0.000022.0	1	1.140	5.3	537.28	2.4	2	'2/10	6917	
5	K.TIEKDK.C	0.000200.0	1	2.090	2.9	488.75	1.6	2	'4/10	7387	
6	R.NAAFAKR.T	0.0000020.0	1	5.460	1.2	510.77	3.2	2	'5/12	7485	
7	K.KAKPARTHWDML MER.R	0.202000000000100.0	1	0.700	2.6	1186.57	2.8	2	'3/28	19104	
8	K.LADTVK.V	0.000002.0	1	2.690	4.1	445.23	5.5	2	'4/10	6286	
9	-MSNESLANLLKEER. R	0.10000000002000.0	1	0.670	3.3	473.98	1.3	4	'2/26	7967	
10	K.ISNLK.N	0.00002.0	1	7.260	1.7	409.23	1.8	2	'3/8	5306	
11	R.ALAEGLTK.R	0.00000002.0	1	0.380	7.2	523.28	0.3	2	'4/14	10206	
12	K.KVMPRLSAGR.V	0.2010000000.0	1	5.270	2	687.37	0.9	2	'3/18	16656	
13	R.GLDSSLRRSGWK.G	0.00000000002.0	1	4.030	2.3	759.39	6.1	2	'3/20	19230	
14	R.MSEVIGDVAKVGA ER.I	0.00000000020000.0	1	0.700	3.5	601.97	2.7	3	'4/28	14793	
15	R.KAEKVIIDR.A	0.000200000.0	1	1.040	6.5	657.8	6.2	2	'2/16	9590	

						7				
16	K.MLGEAAGKPDLK.K	0.000000000002.0	1	2.330	3.3	736.87	2.6	2	'3/22	11312
17	K.GIDGDLINEIFDLLYQKR.L	0.000000000000000020.0	1	13.410	0.27	1183.11	3.9	2	'4/34	29961
18	K.VDVAPIGDVK.W	0.0000000002.0	1	0.170	3.6	628.33	5.6	2	'3/18	19323
19	K.STMQVAQK.L	0.00100002.0	1	2.180	1.1	576.27	1.3	2	'3/14	9561
20	K.AKELVSEANSEAGKVR.I	0.0200000000000000200.0	1	1.080	3.4	725.36	1.3	3	'3/30	22514
21	R.LKPGVGIVVDLGKV.V	0.02000000000002.0	1	0.170	3.4	890.99	6.1	2	'3/24	22614
22	K.KAVIDAKR.G	0.00000020.0	1	10.950	0.66	572.33	4.1	2	'4/14	6125
23	R.GGKVFNR.T	0.0020000.0	1	5.480	1.2	510.77	3.1	2	'3/12	7485
24	K.MPRIRK.V	0.100002.0	1	0.480	9.5	530.29	0.0	2	'2/10	13613
25	R.VFDLFPMTAHVECVAILEPAAK.G	0.000000000000000000002.0	1	0.730	3.9	1351.17	0.9	2	'2/42	29741
26	K.SWLPSVSLLK.L	0.0000000002.0	1	1.090	6.4	686.88	0.7	2	'3/18	15663
27	K.ATVKGGLGKLR.E	0.00000000200.0	1	1.060	3	671.89	2.2	2	'3/20	22747
28	K.GASVLK.Q	0.000002.0	5	12.630	0.5	409.23	1.8	2	'4/10	5306
29	K.AIAEVKRA.A	0.0000020.0	1	4.260	2.7	515.29	3.9	2	'3/12	7508
30	R.VLKAEGLR.V	0.00200000.0	1	2.780	2.8	564.82	2.7	2	'4/14	10583
31	K.SVVKAQVKVGGR.G	0.00020000000.0	1	1.110	4.1	735.92	1.5	2	'2/22	11701
32	R.MLVSDMAGRASIELK.G	0.10000000000000002.0	1	3.420	1.8	940.46	2.1	2	'2/28	30483
		36								

- # Serial (sequential) number for peptide.
Sequence Assigned peptide sequence. Periods (".") delimit the sequence for internal peptides.
PTM Site Location of the post-translational modification (PTM) in the peptide.
Modification codes: [1] Oxidation (M); [2] pupylation (K)
Nr. Scans The number of MS/MS scans that were matched to this peptide.
Mascot Score Score given to this peptide/spectrum match by Mascot.
Expectation The number of matches with equal or better scores that are expected to occur by chance alone.
Isolated Mass "Mass" in the Orbitrap analyzer.
Delta Mass Difference between the observed and theoretical masses, in ppm.
Charge State Inferred ionic state of the peptide.
Matched Ions disabled. Number of matched MS/MS ions, as reported by Mascot. NOTE: Temporarily
Scan Nr. MS/MS scan number in the original Xcalibur RAW file.

Reference:

1. Kieser T, Bibb M, Buttner M, Chater K, Hopwood D. The John Innes Foundation; 2000.
2. Vecchione J, Alexander B, Sello J. *Antimicrob. Agents Chemother.* 2009. 53,4673-4677.
3. Gust B., Kieser T., Chater K. (2002) REDIRECT technology: PCR-targeting system in *Streptomyces coelicolor*. http://streptomyces.org.uk/redirect/protocol_V1_4.pdf.